Electronic Supplementary Information

One-Pot Synthesis of Dihydroquinolones by Sequential Reactions of *o*-Aminobenzyl Alcohols with Meldrum's acids.

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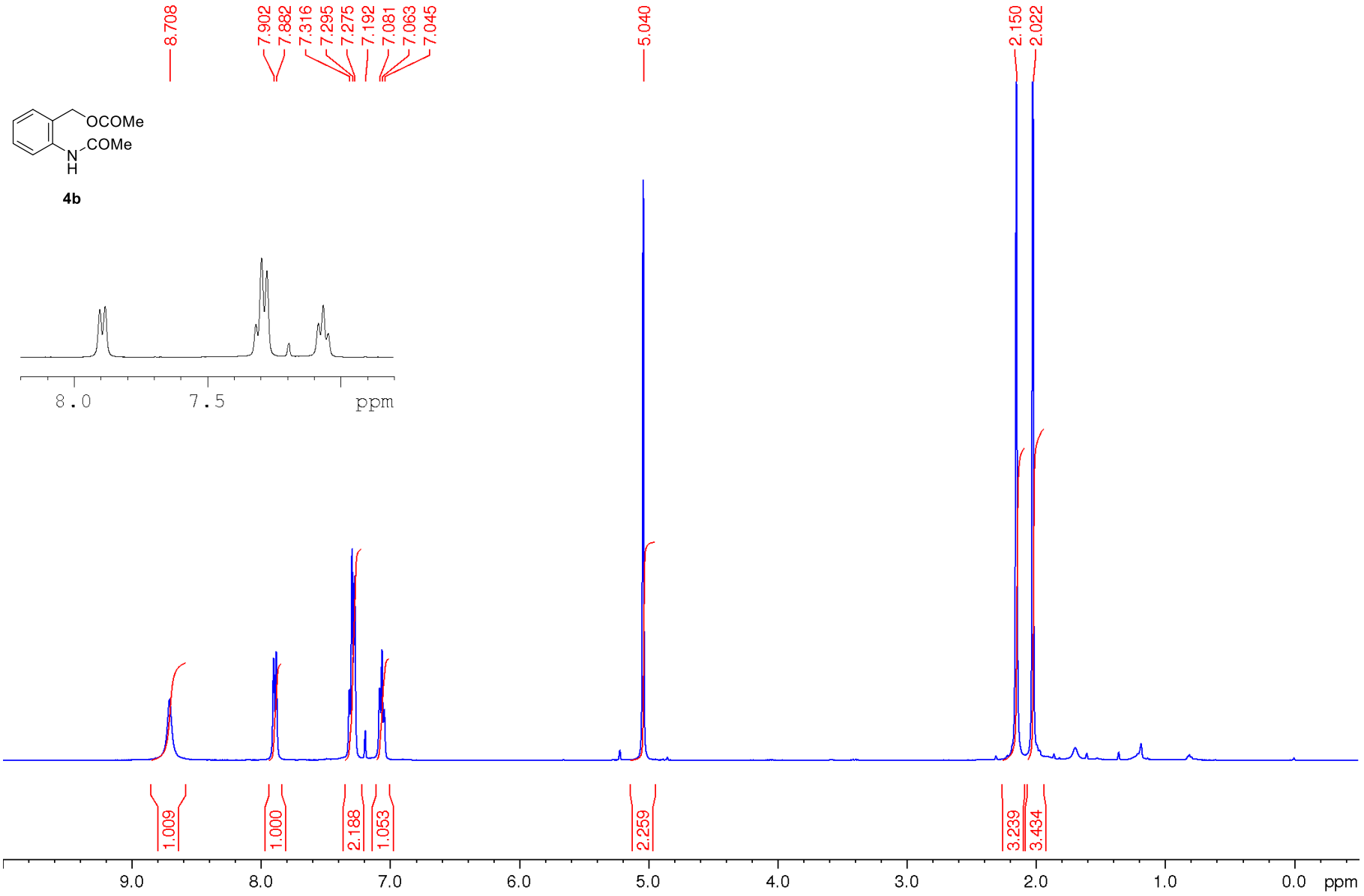
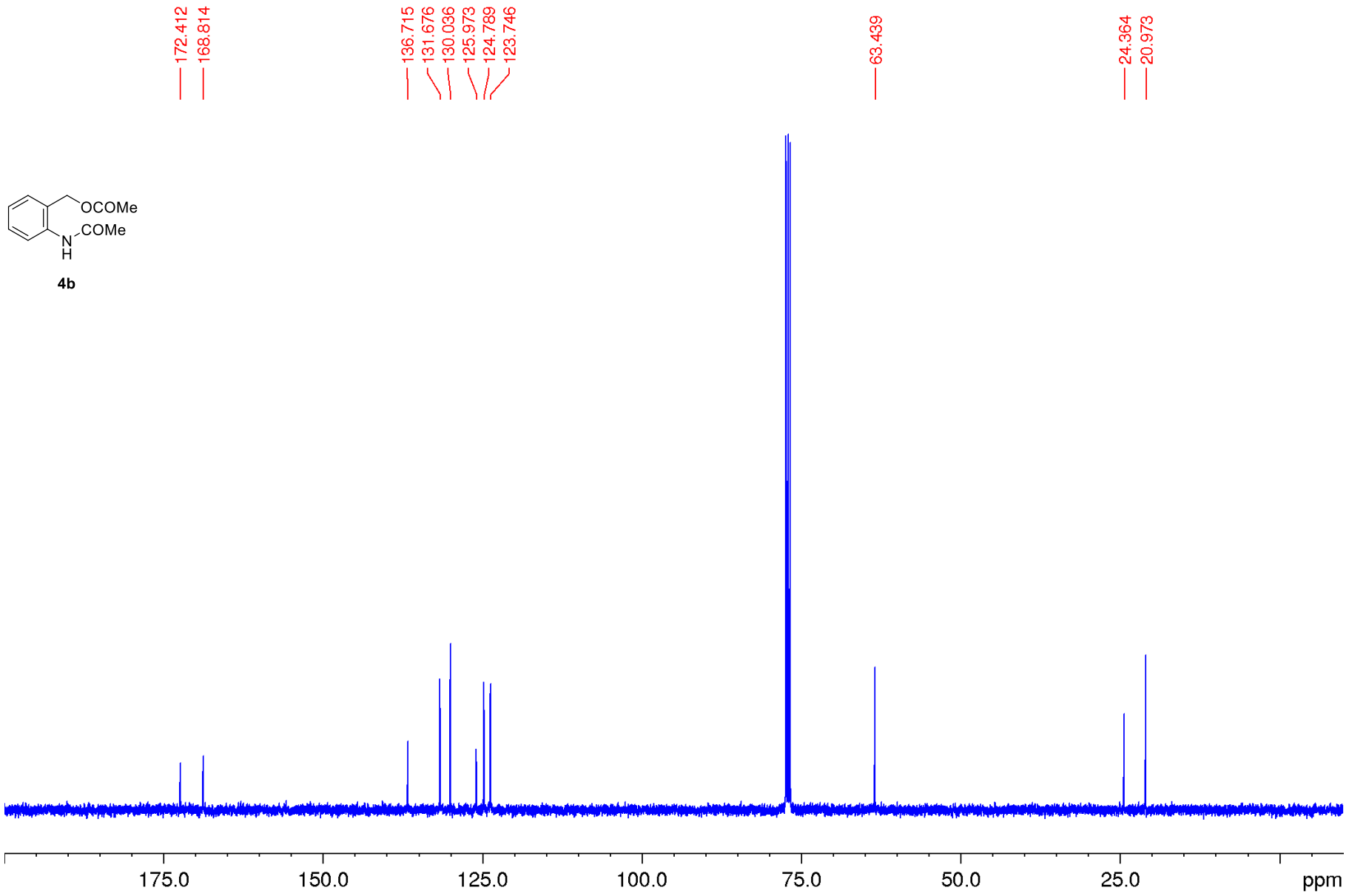
Contents

1. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra for all compounds

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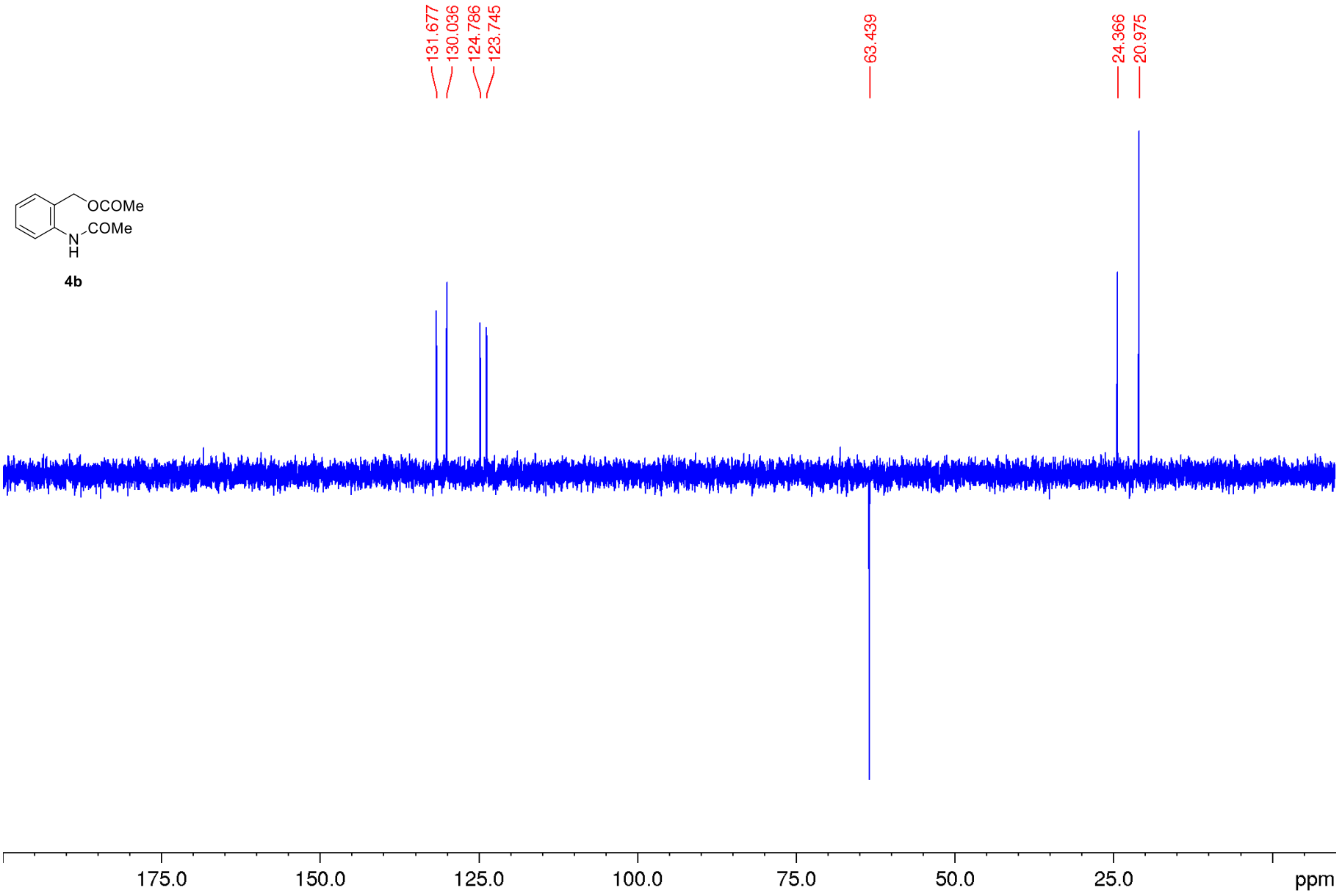
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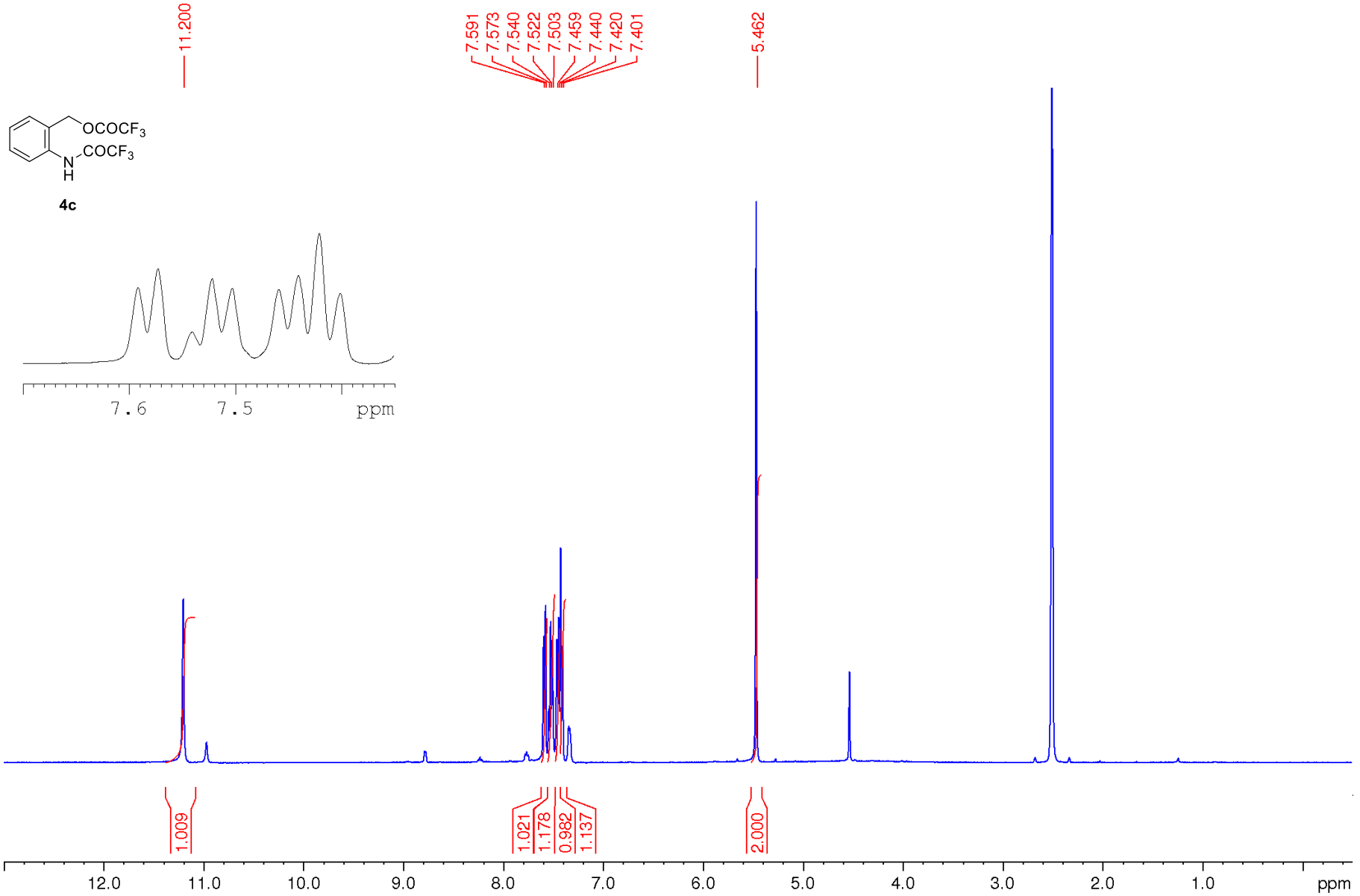
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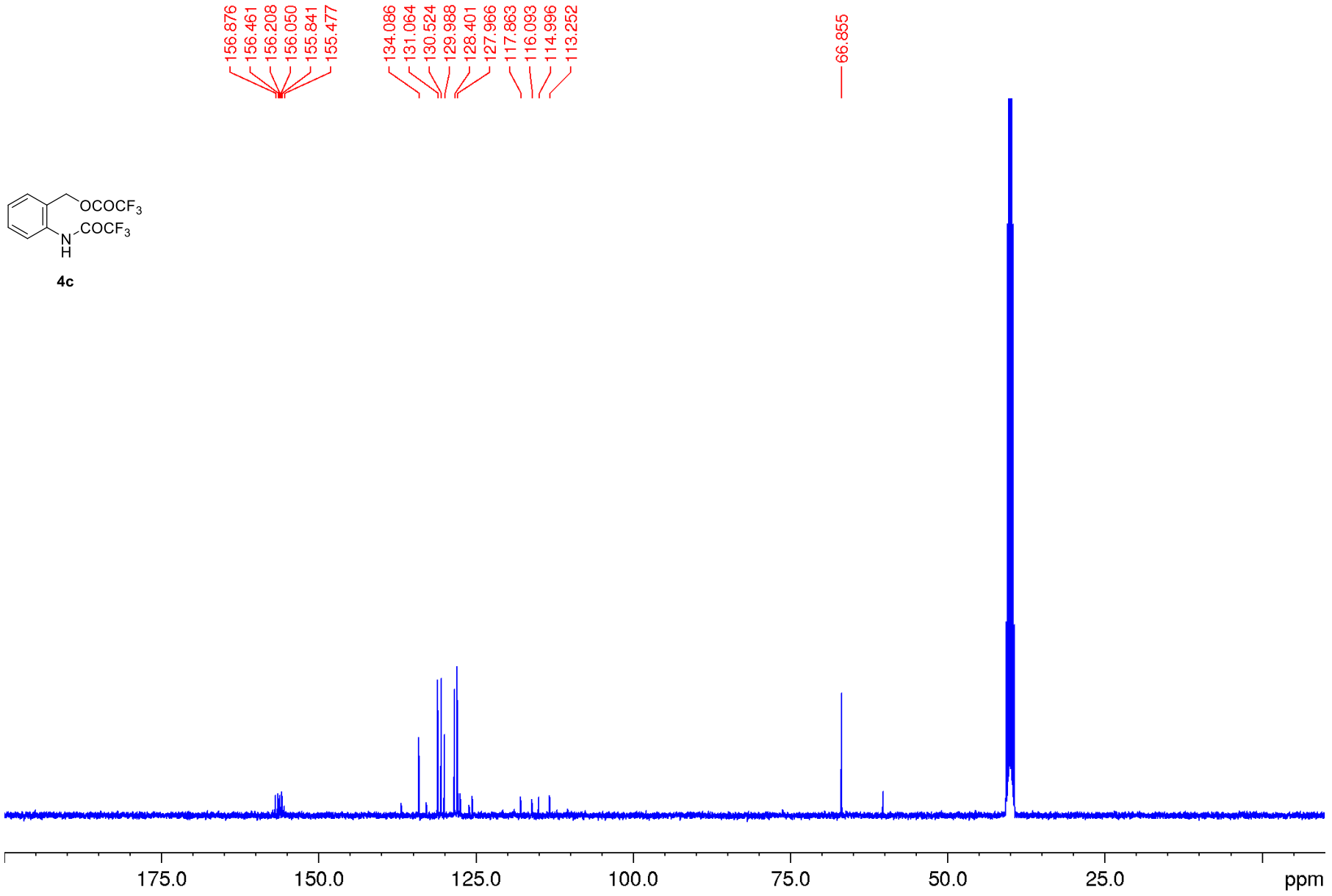
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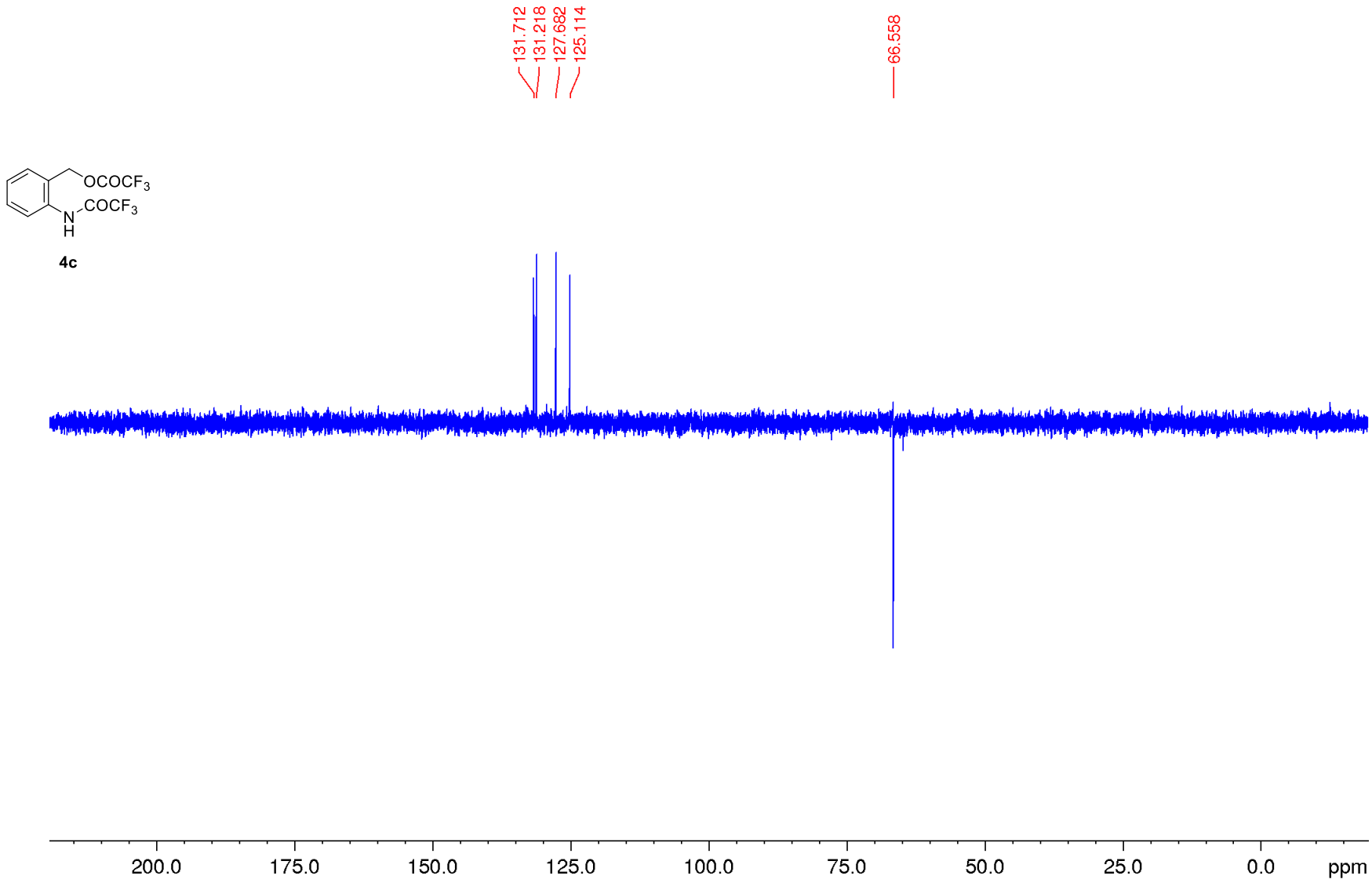
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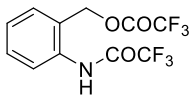

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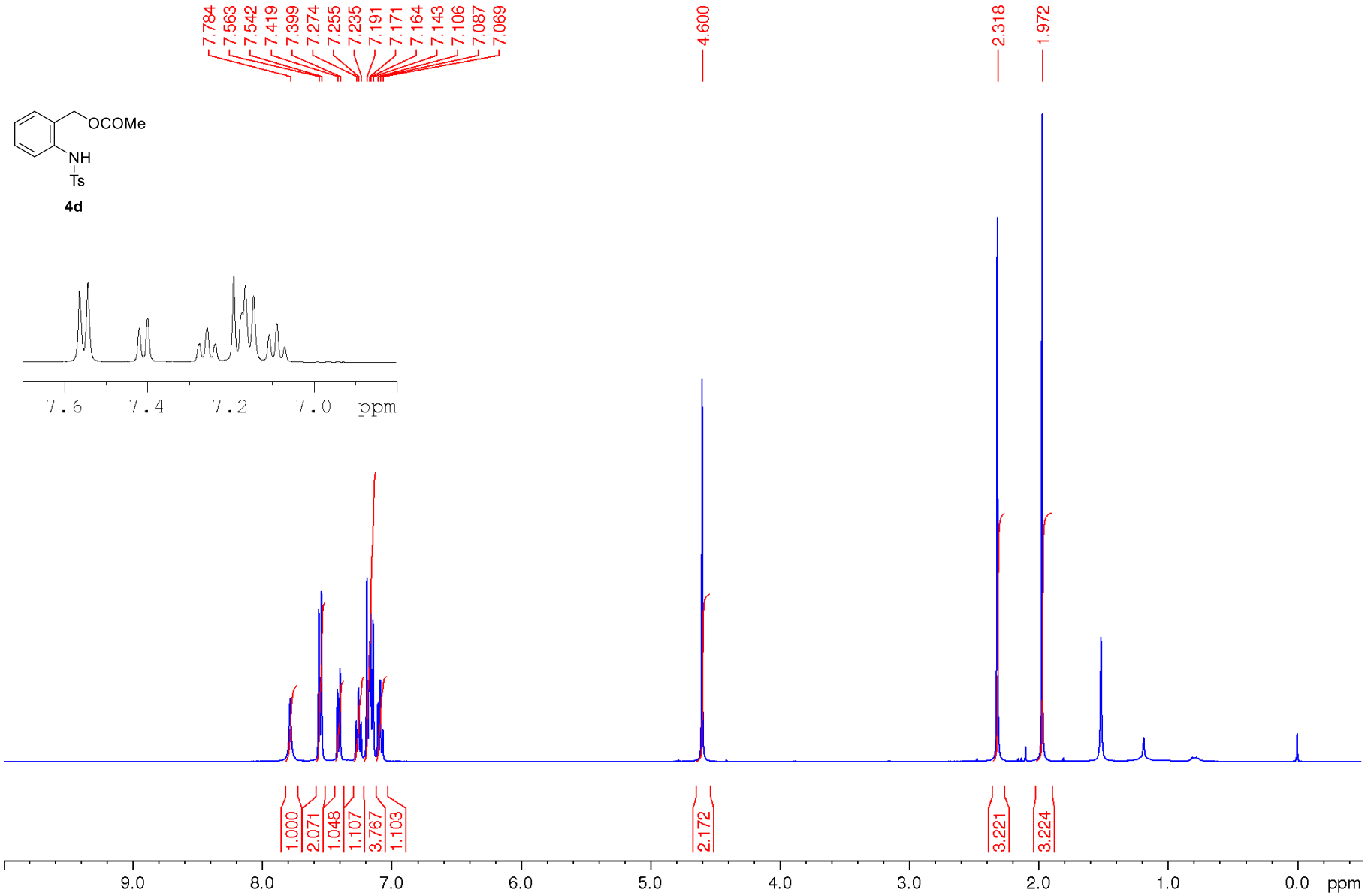
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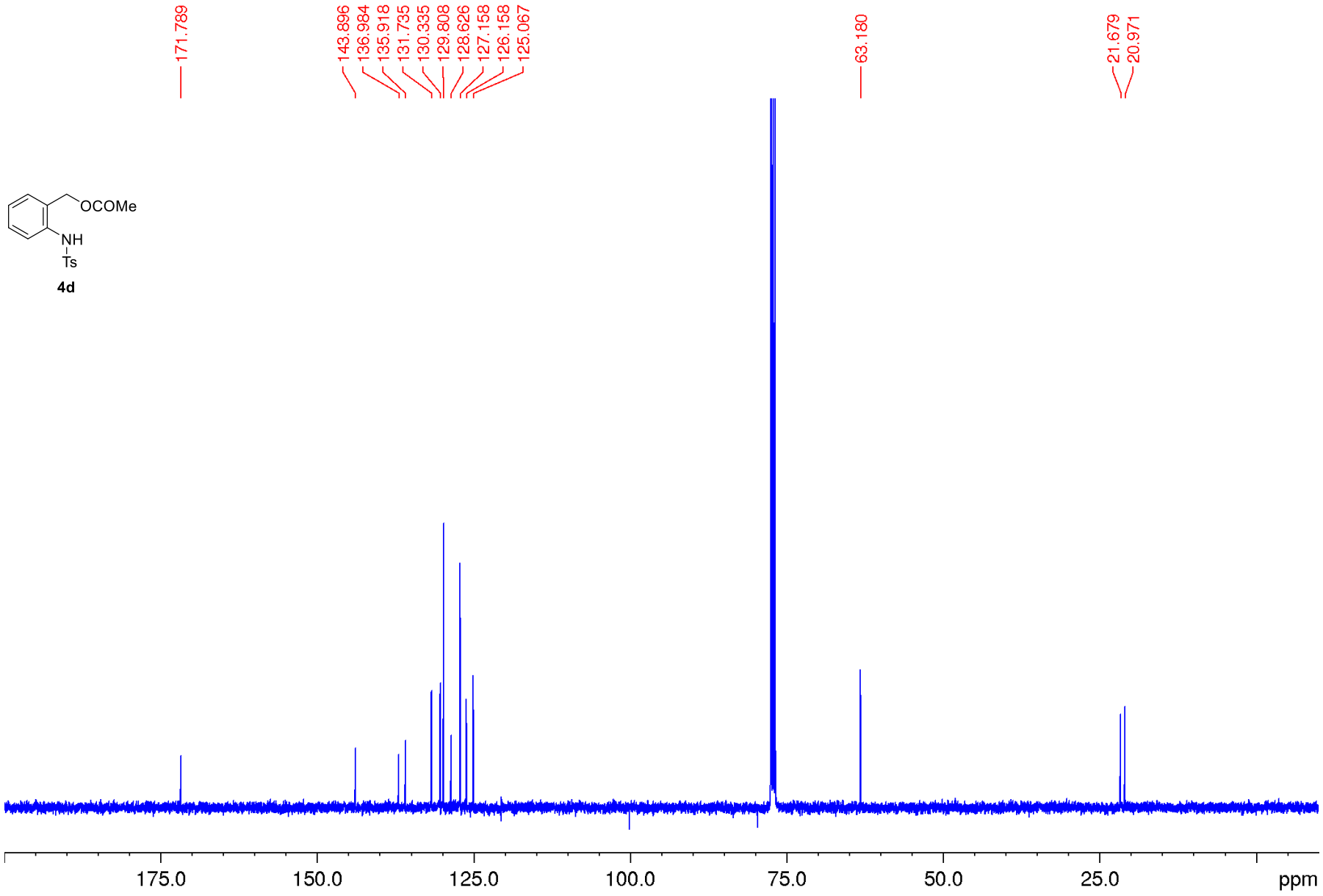
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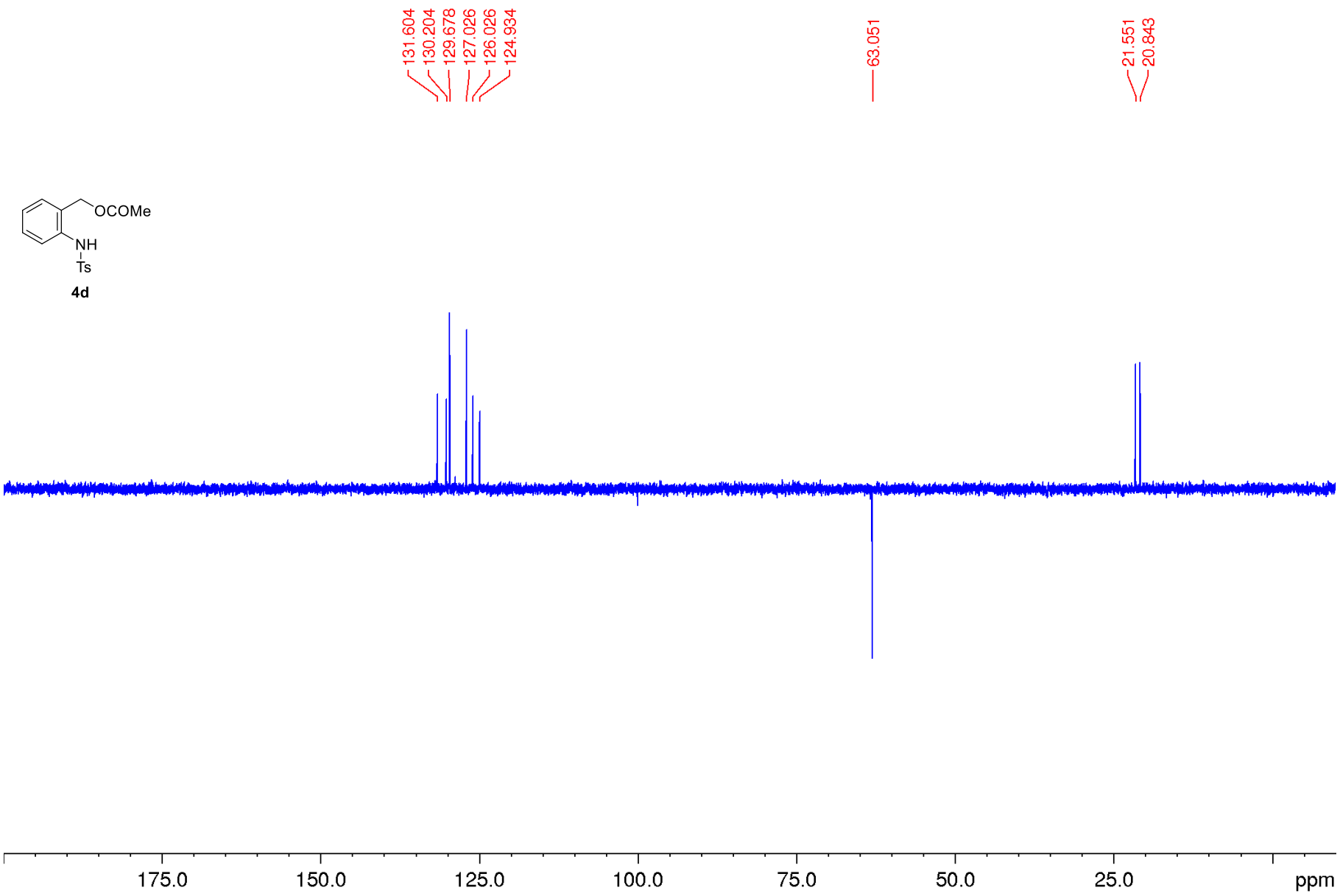
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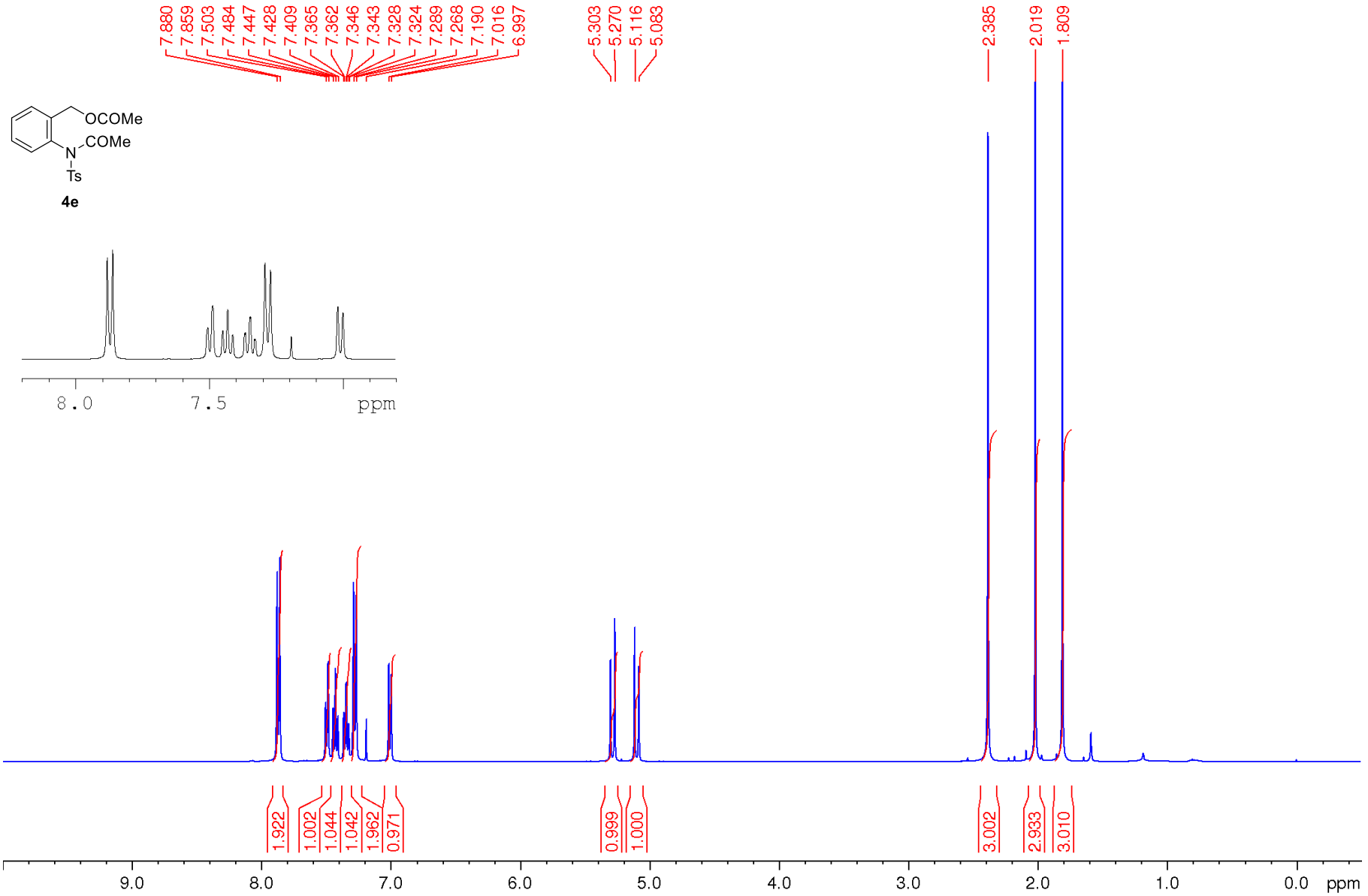
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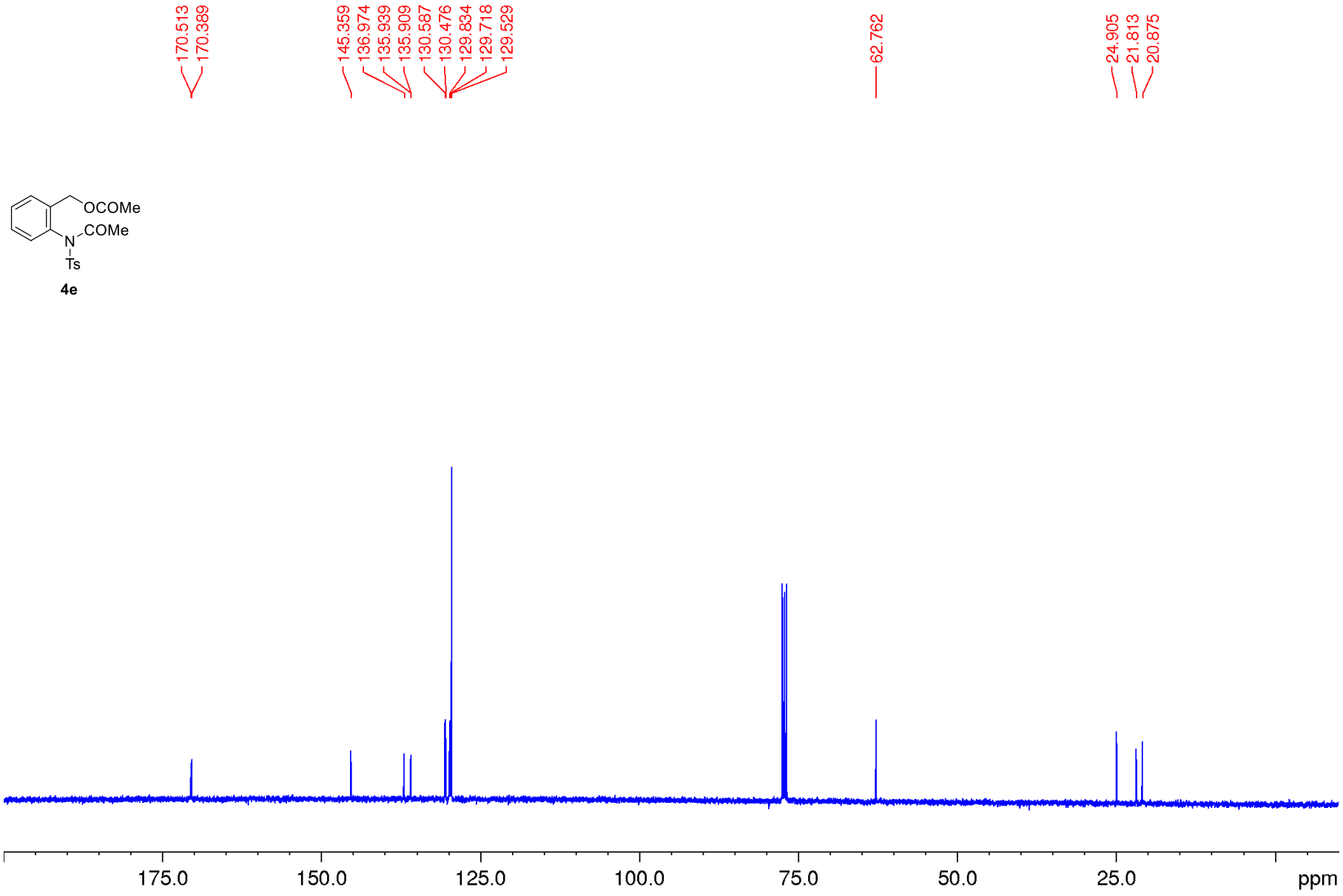
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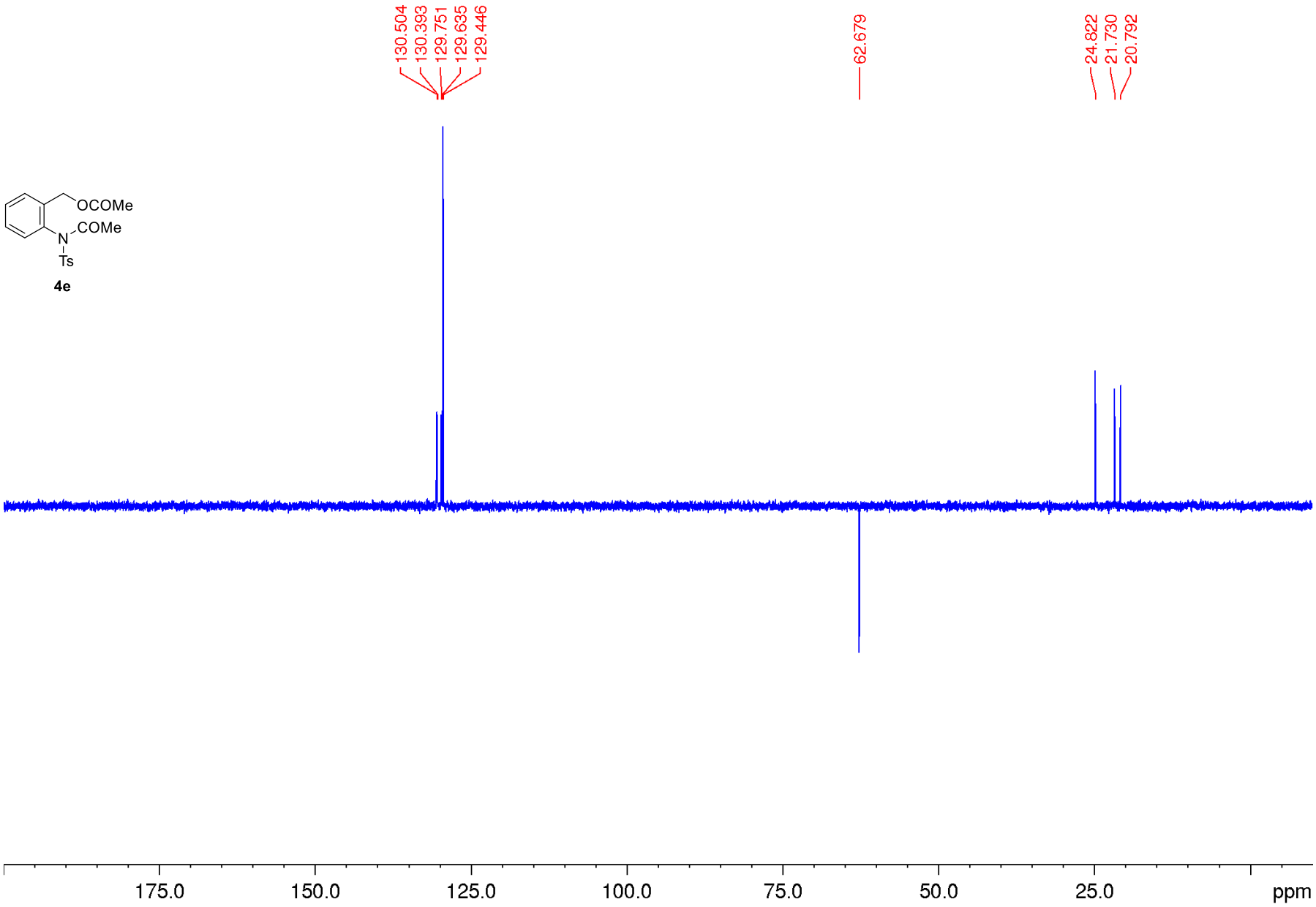
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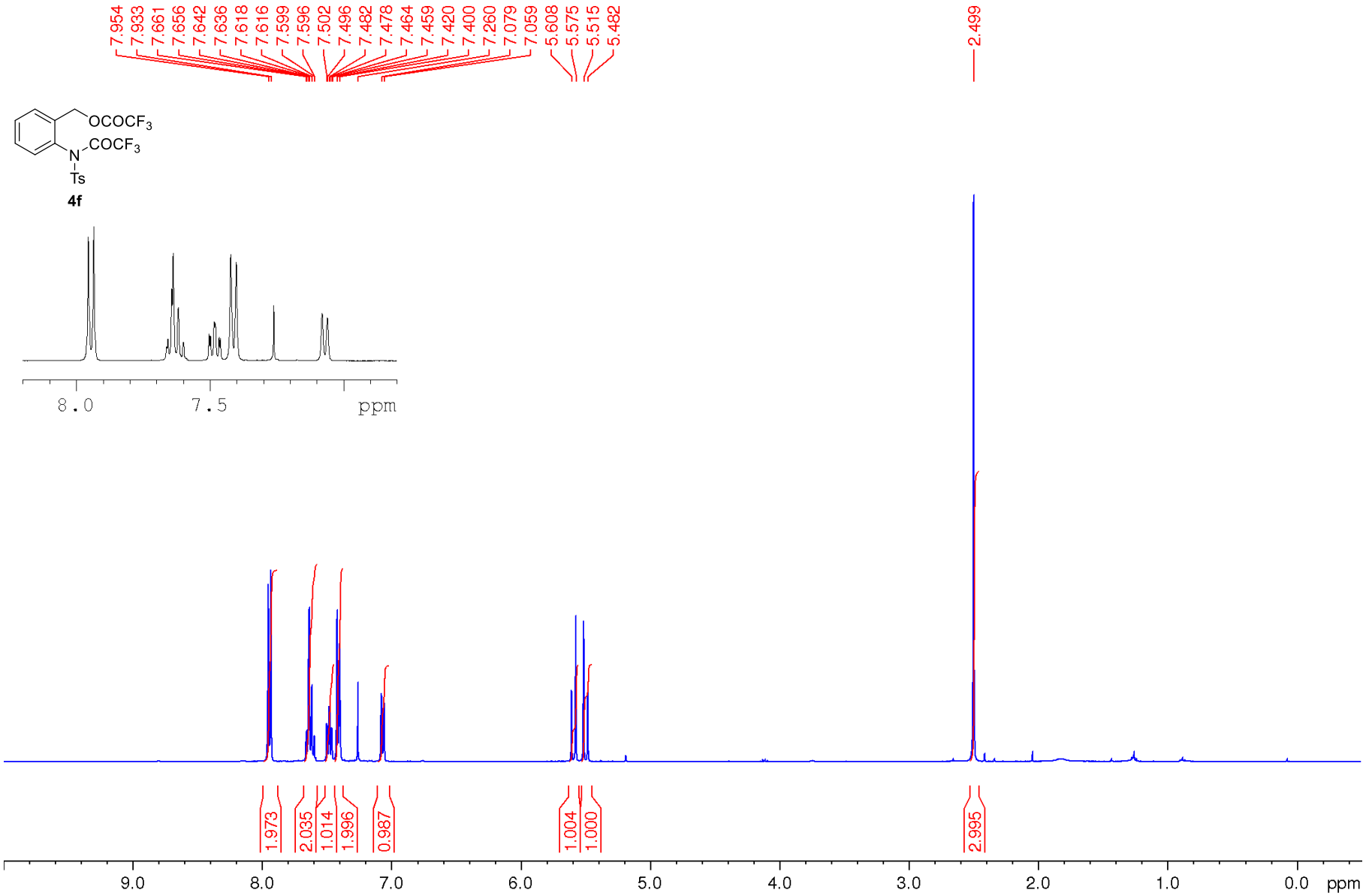
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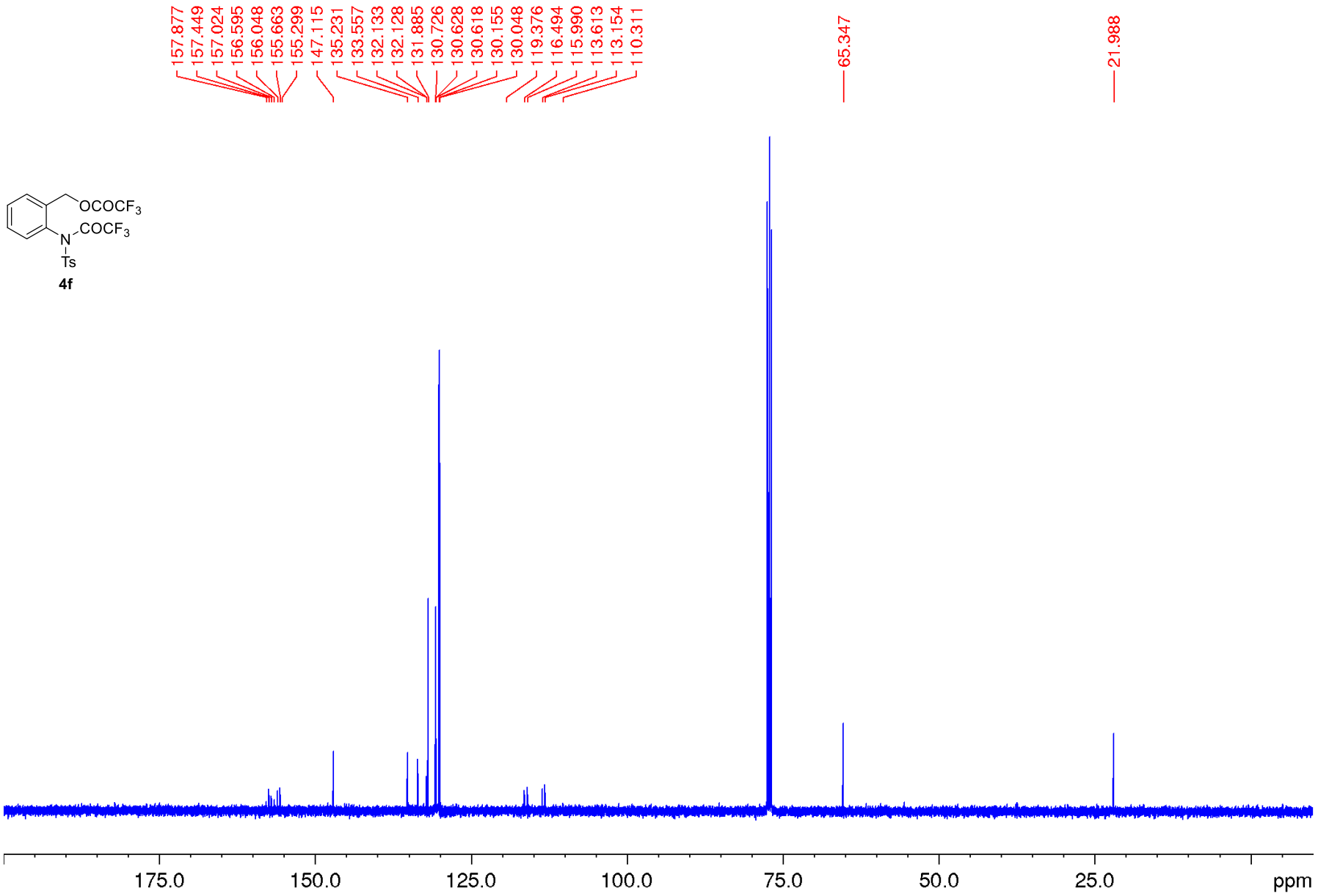
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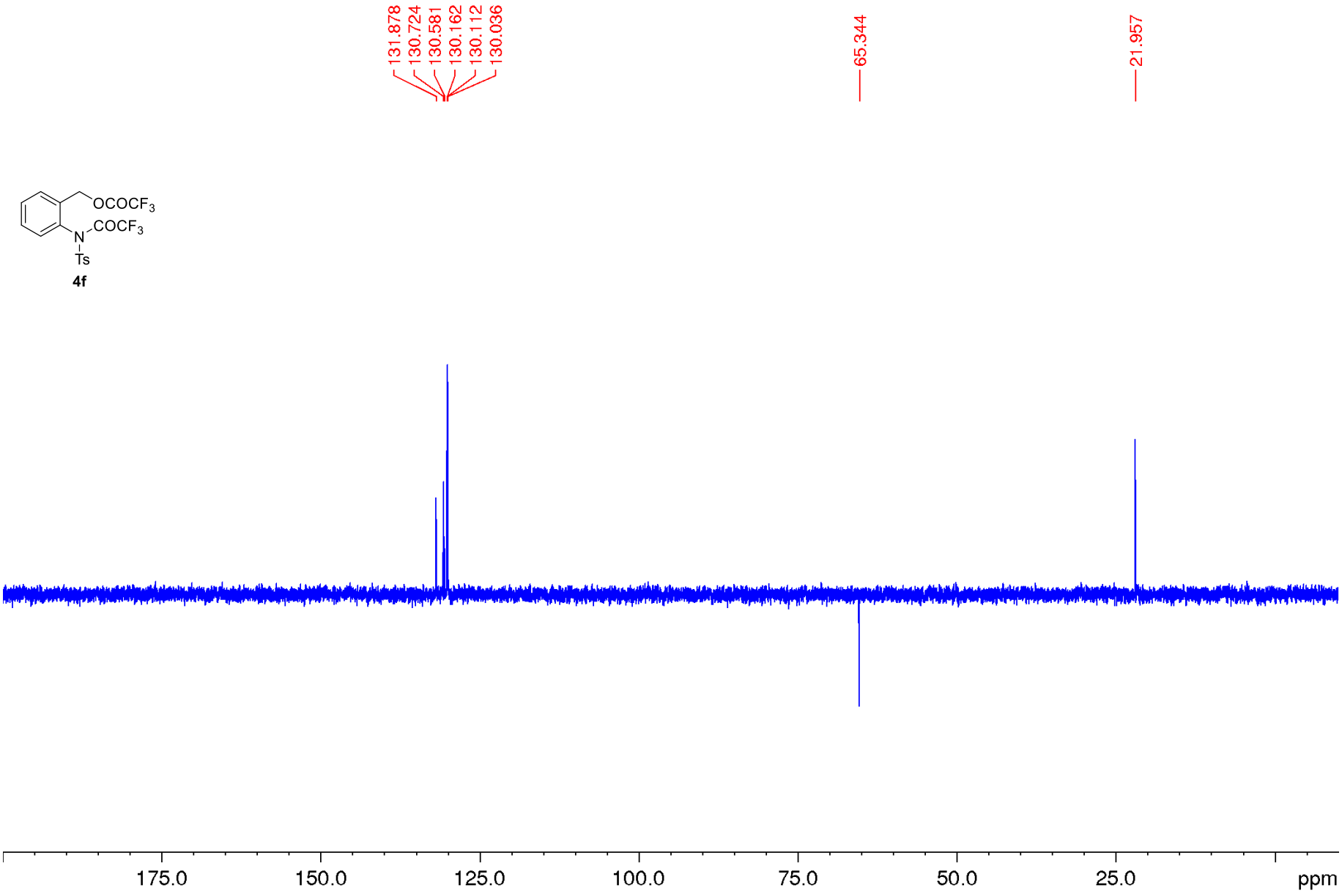
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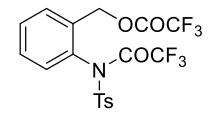

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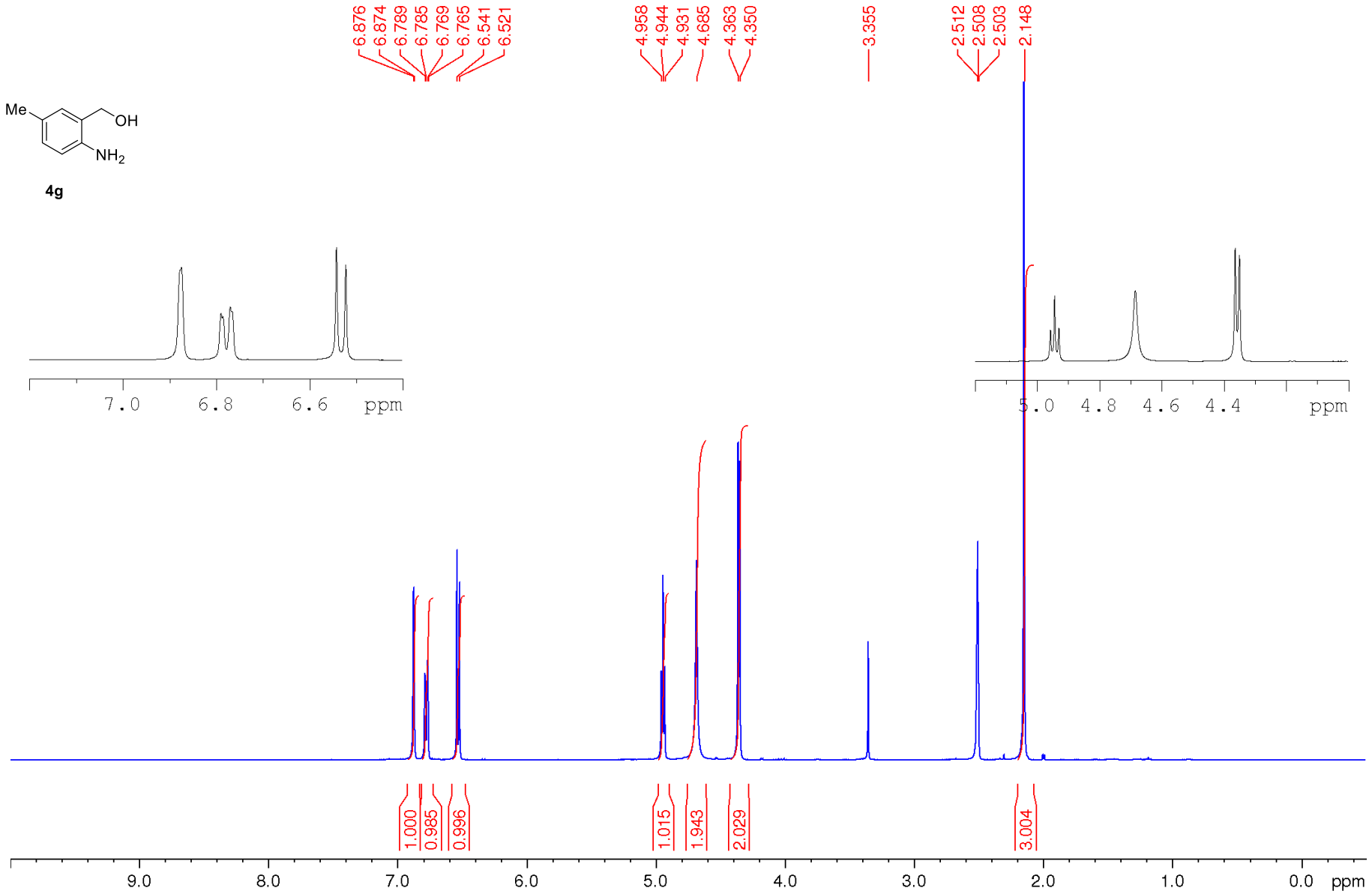
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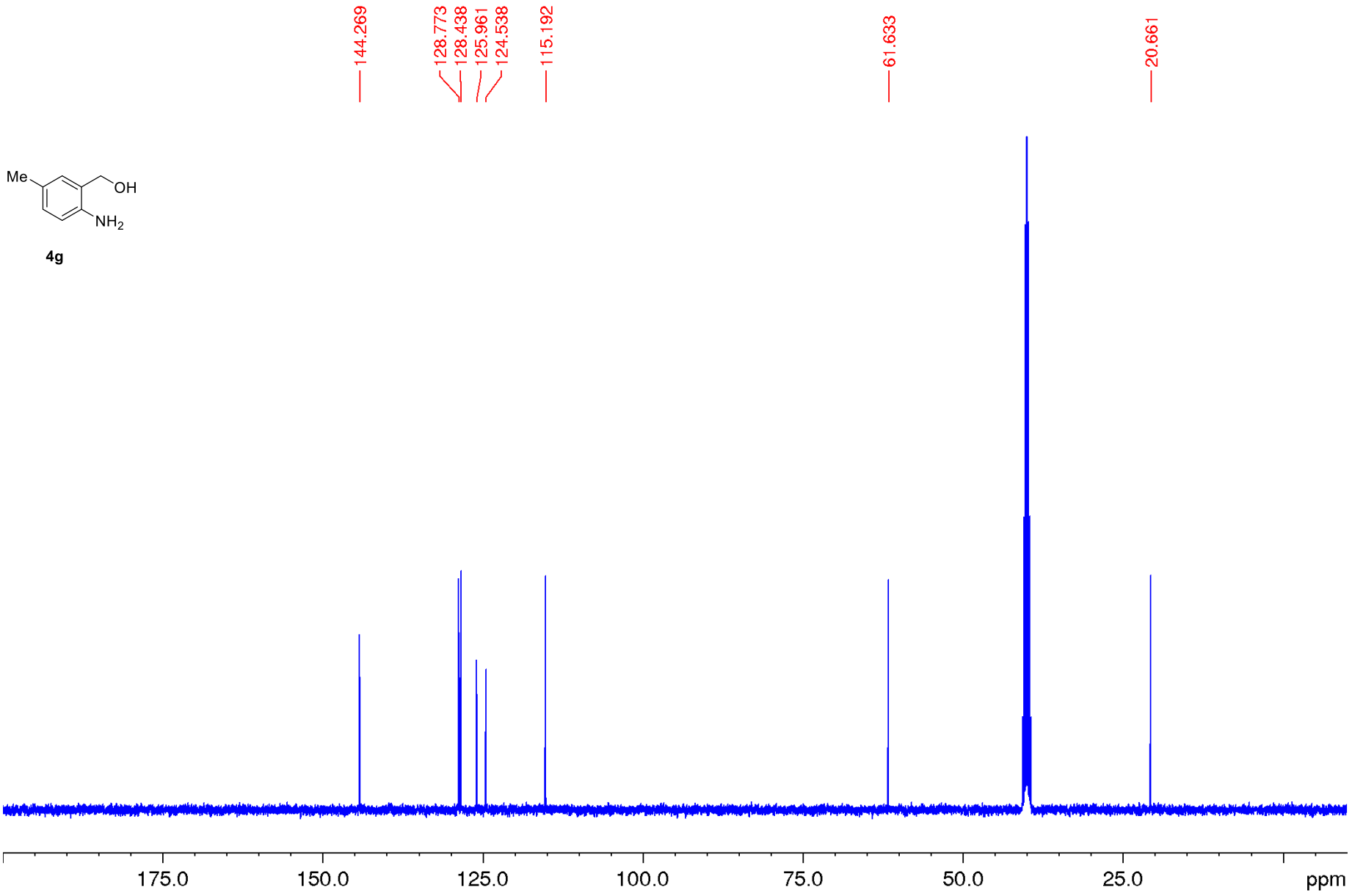
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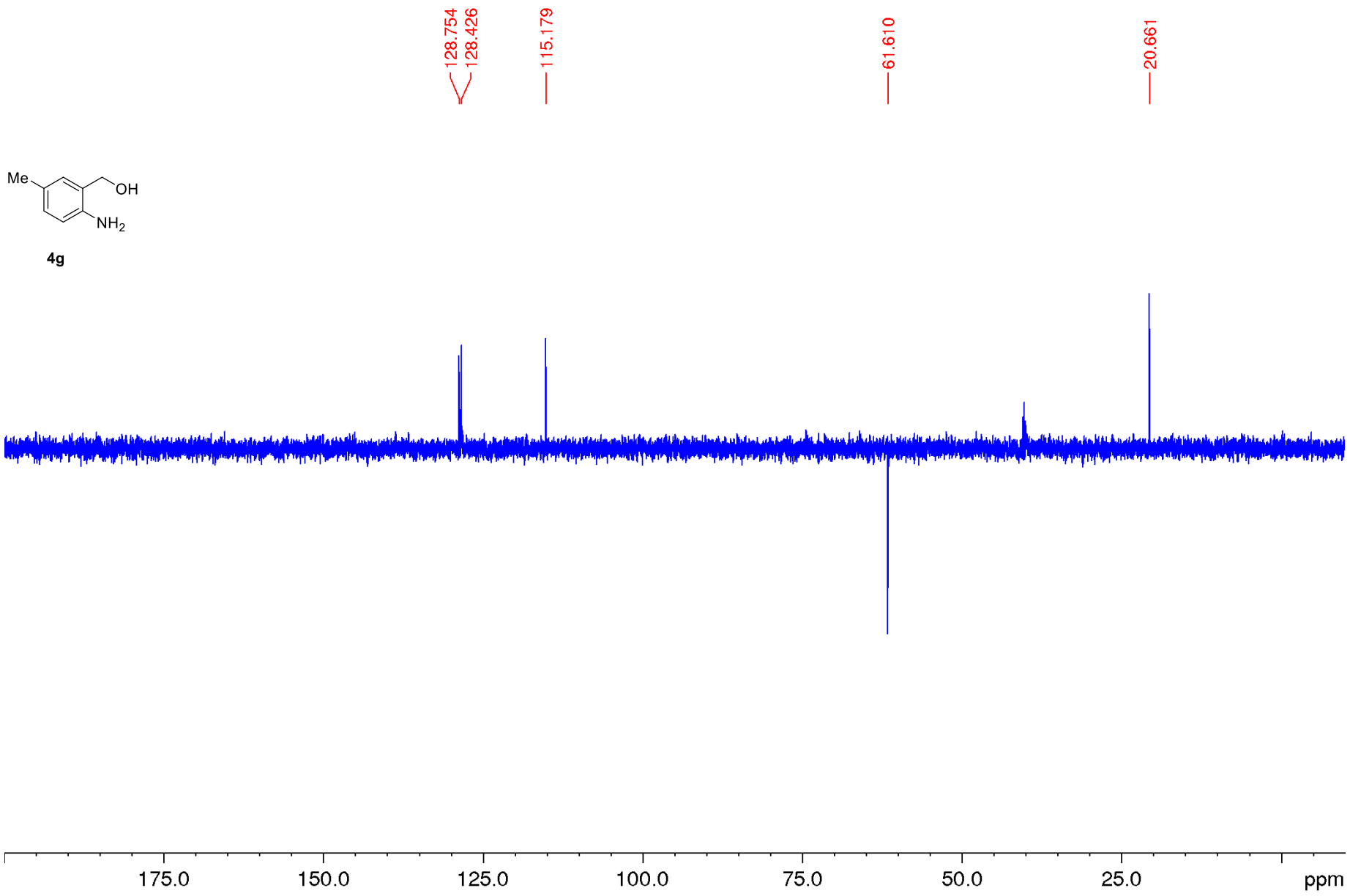
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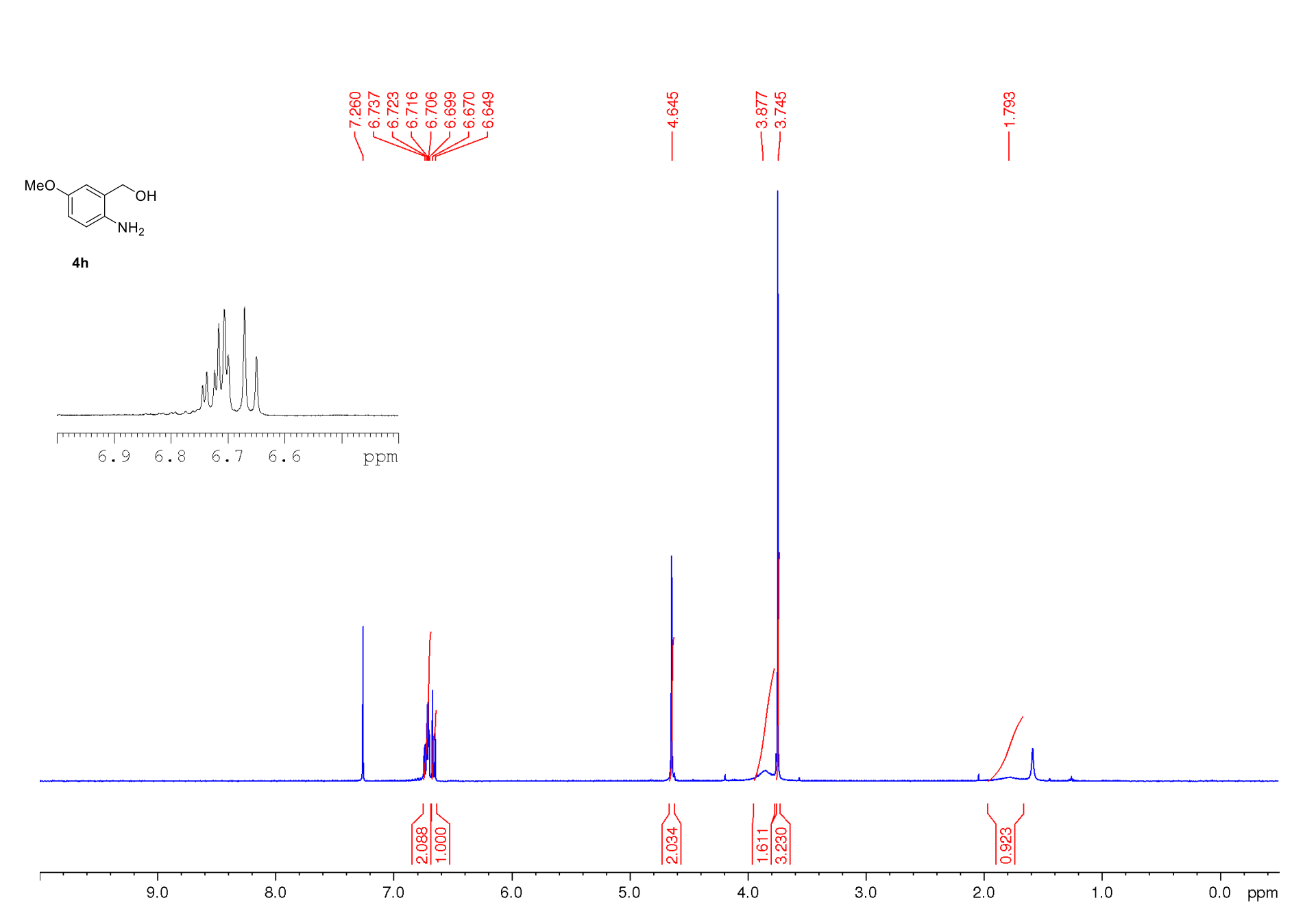
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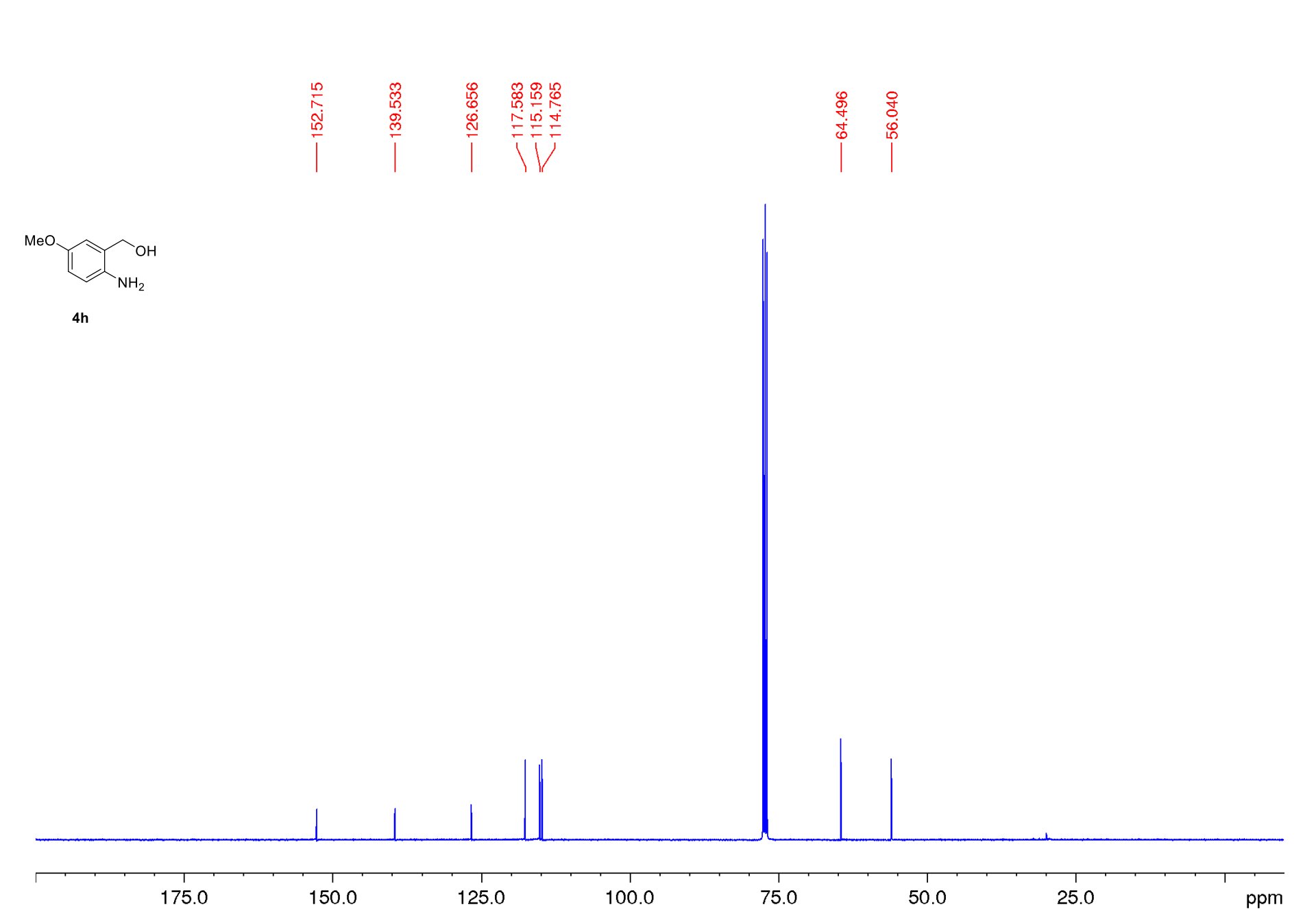
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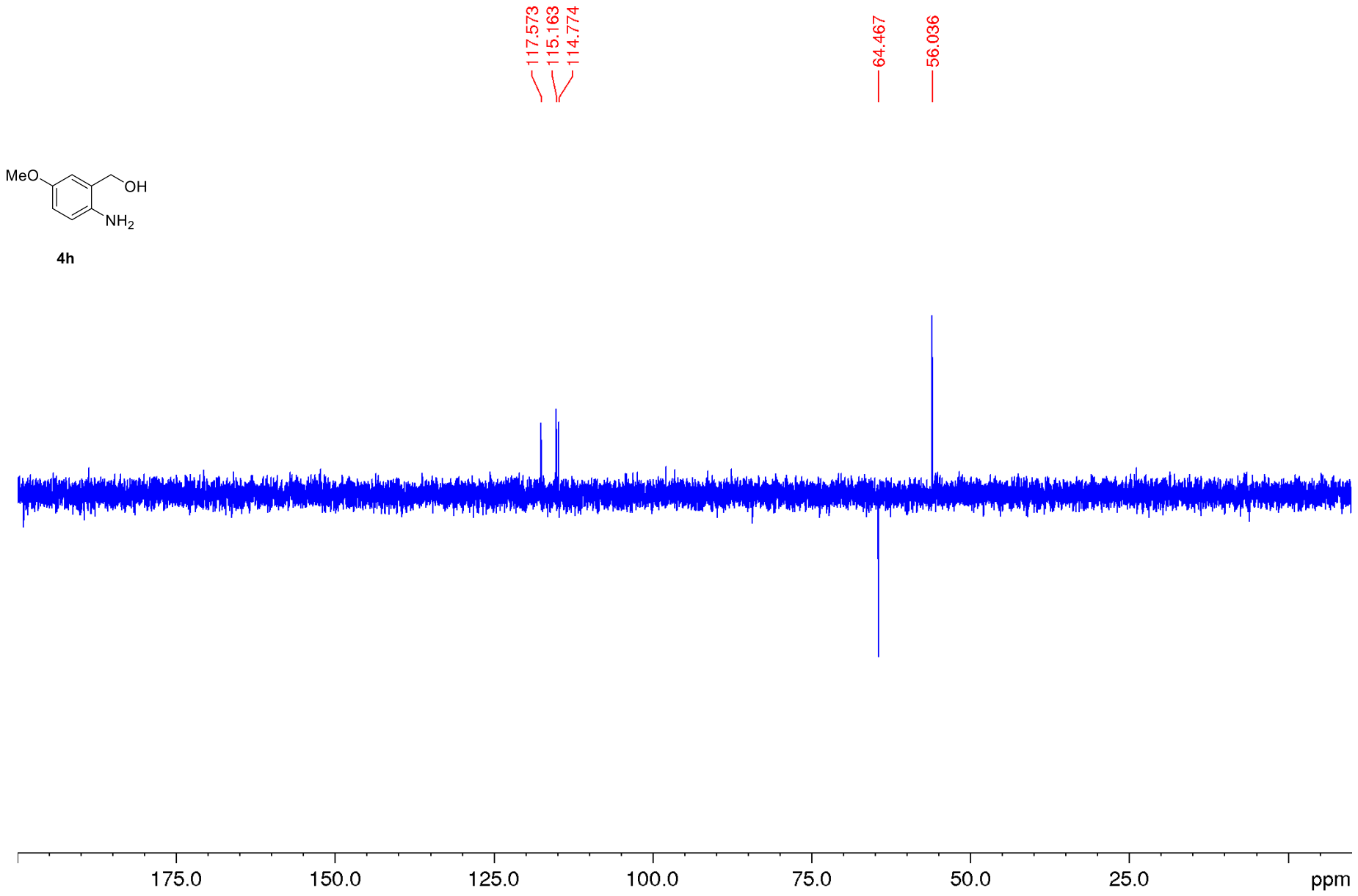
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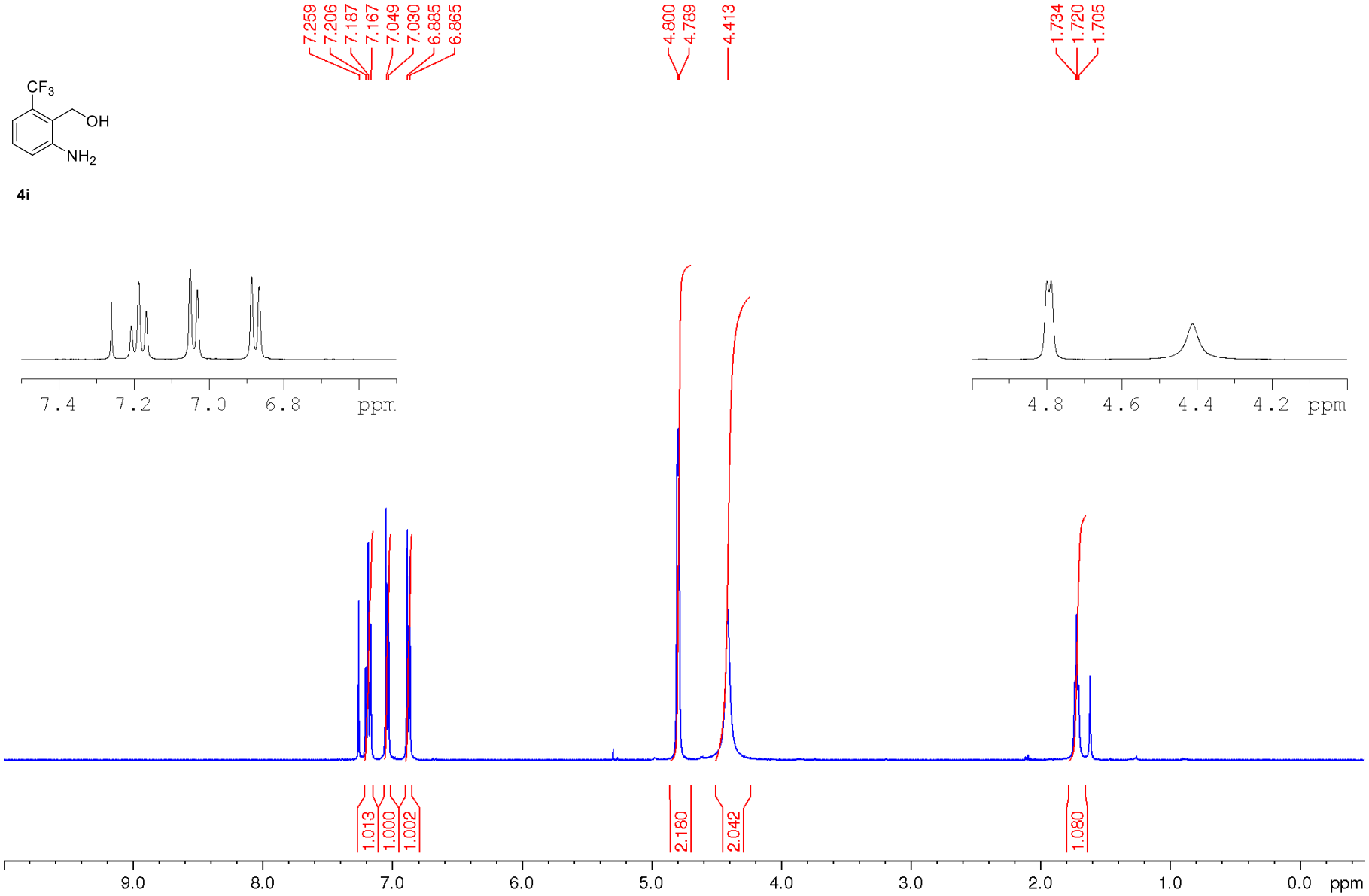
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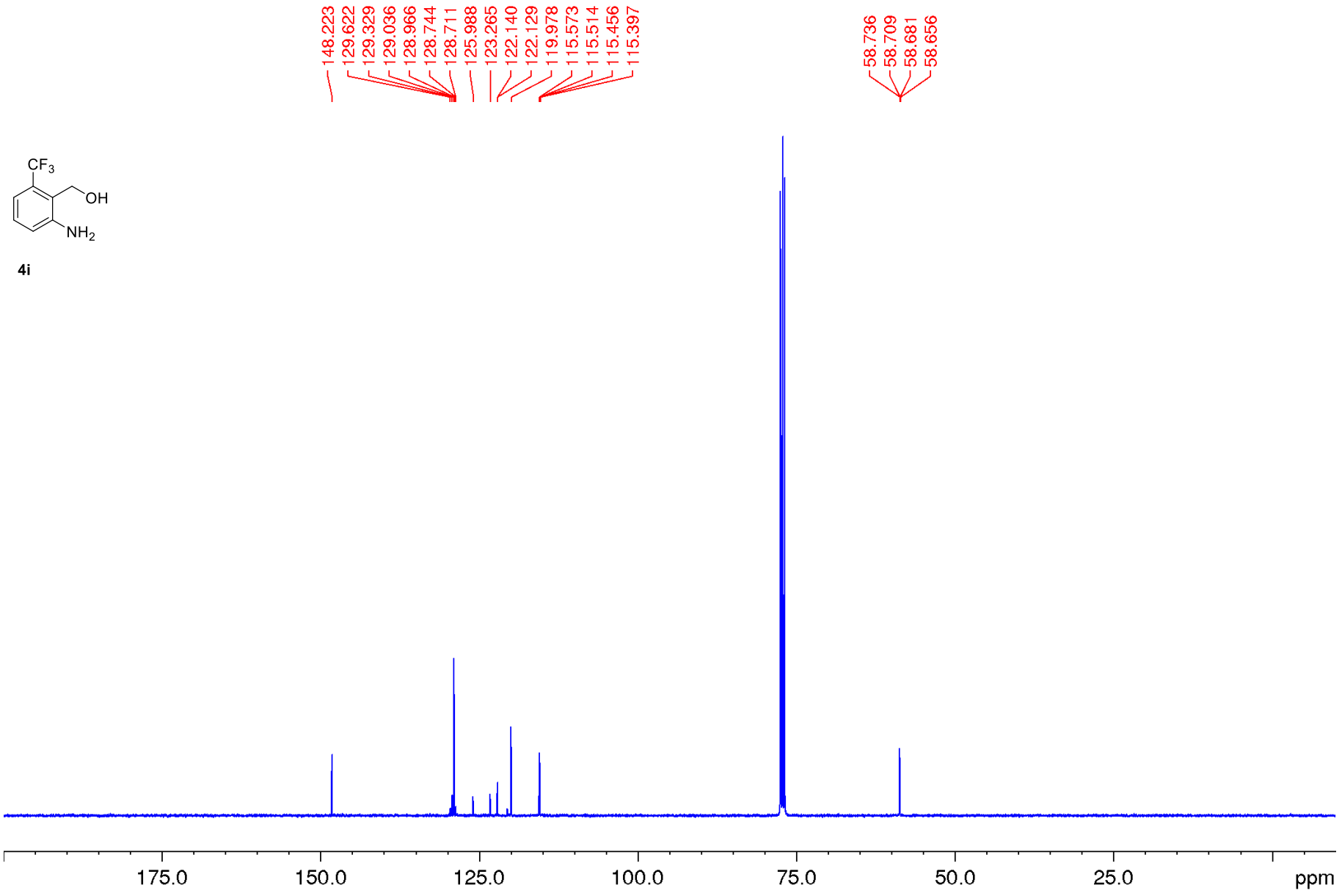
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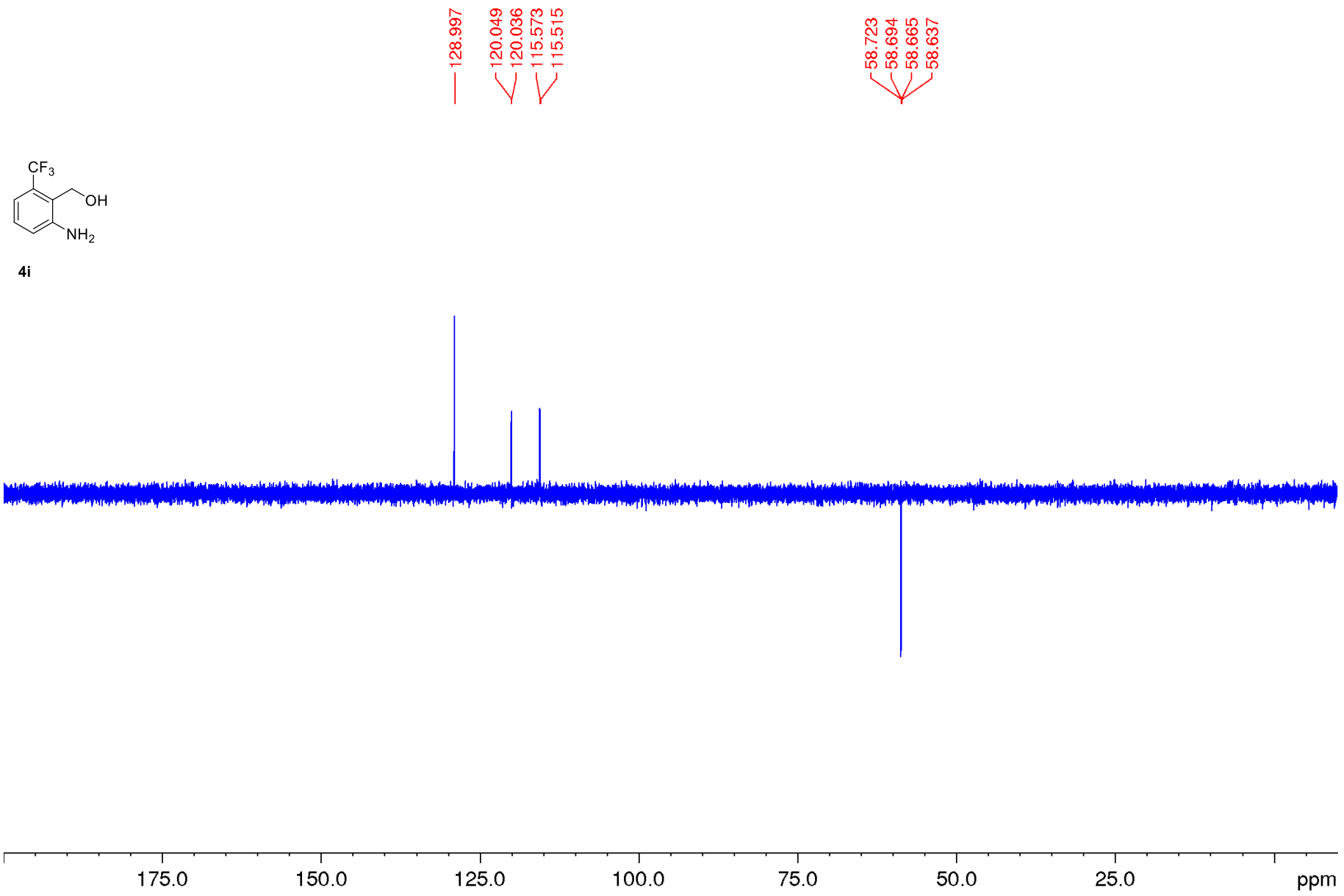
4i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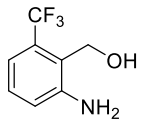

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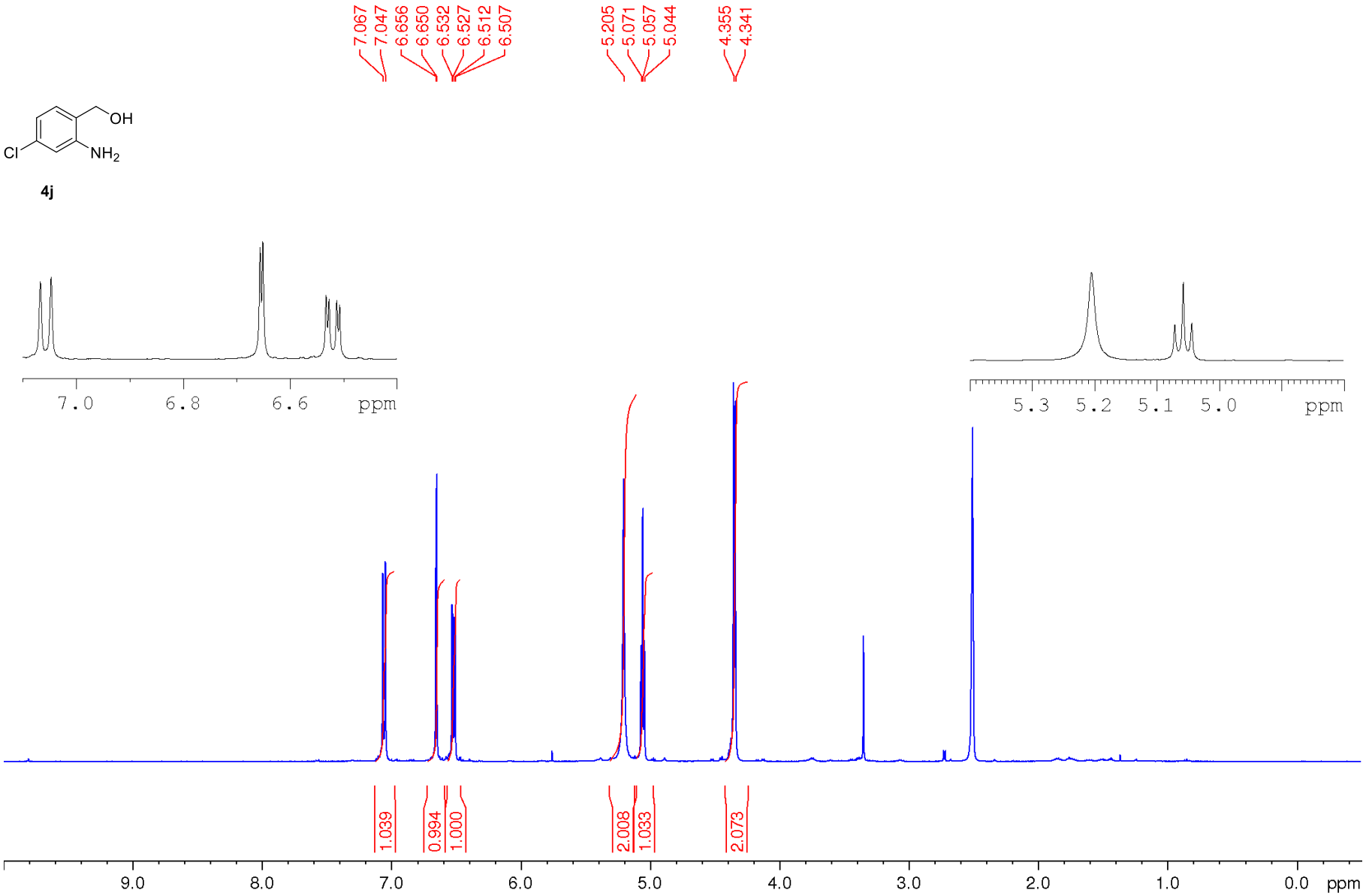
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NH2
4j
7.0
6.8
6.6
ppm
5.3
5.2
5.1
5.0
ppm
1.039
0.994
1.000
2.008
1.033
2.073
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8.0
7.0
6.0
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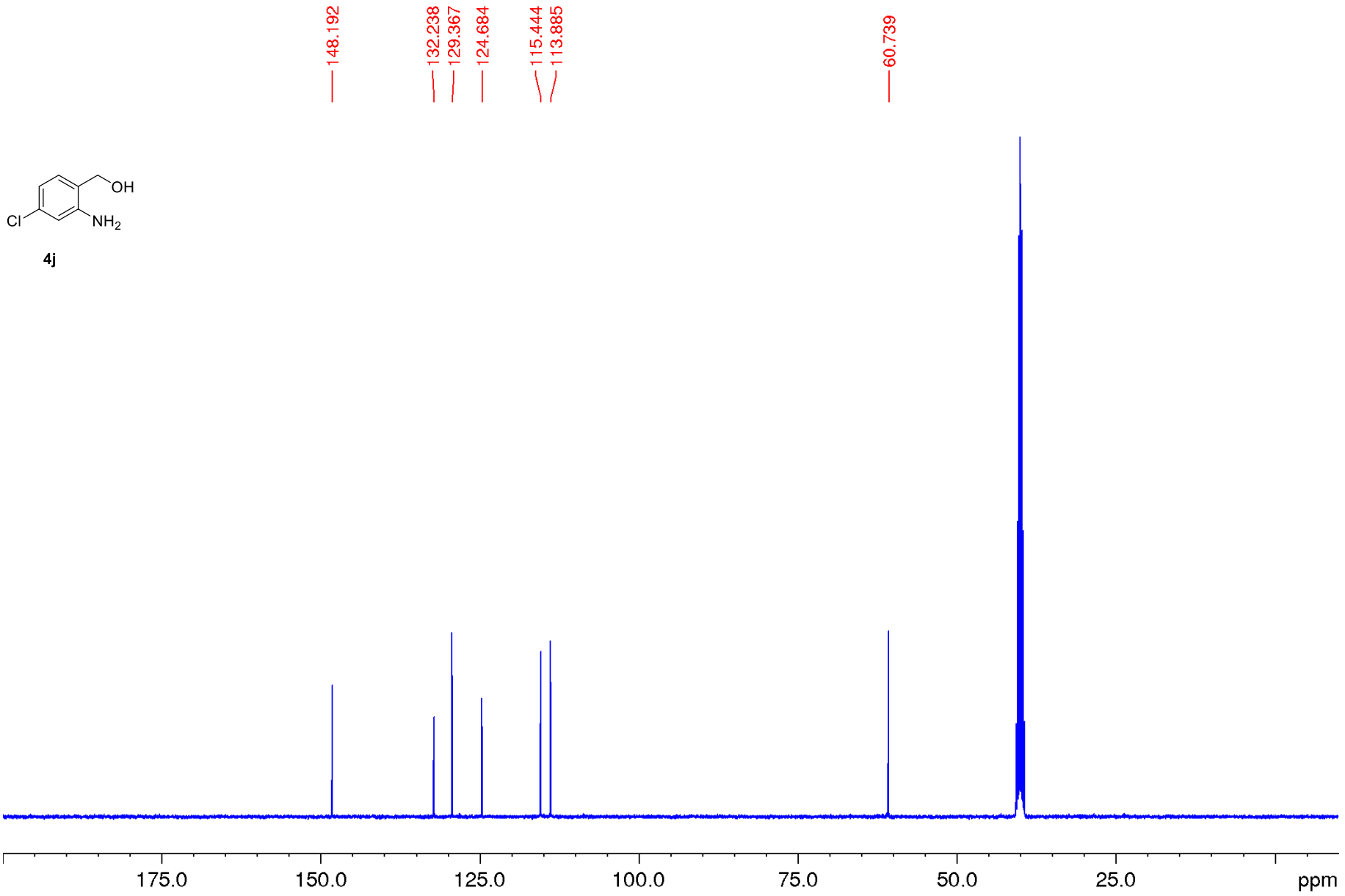
4.0
3.0
2.0
1.0
0.0
ppm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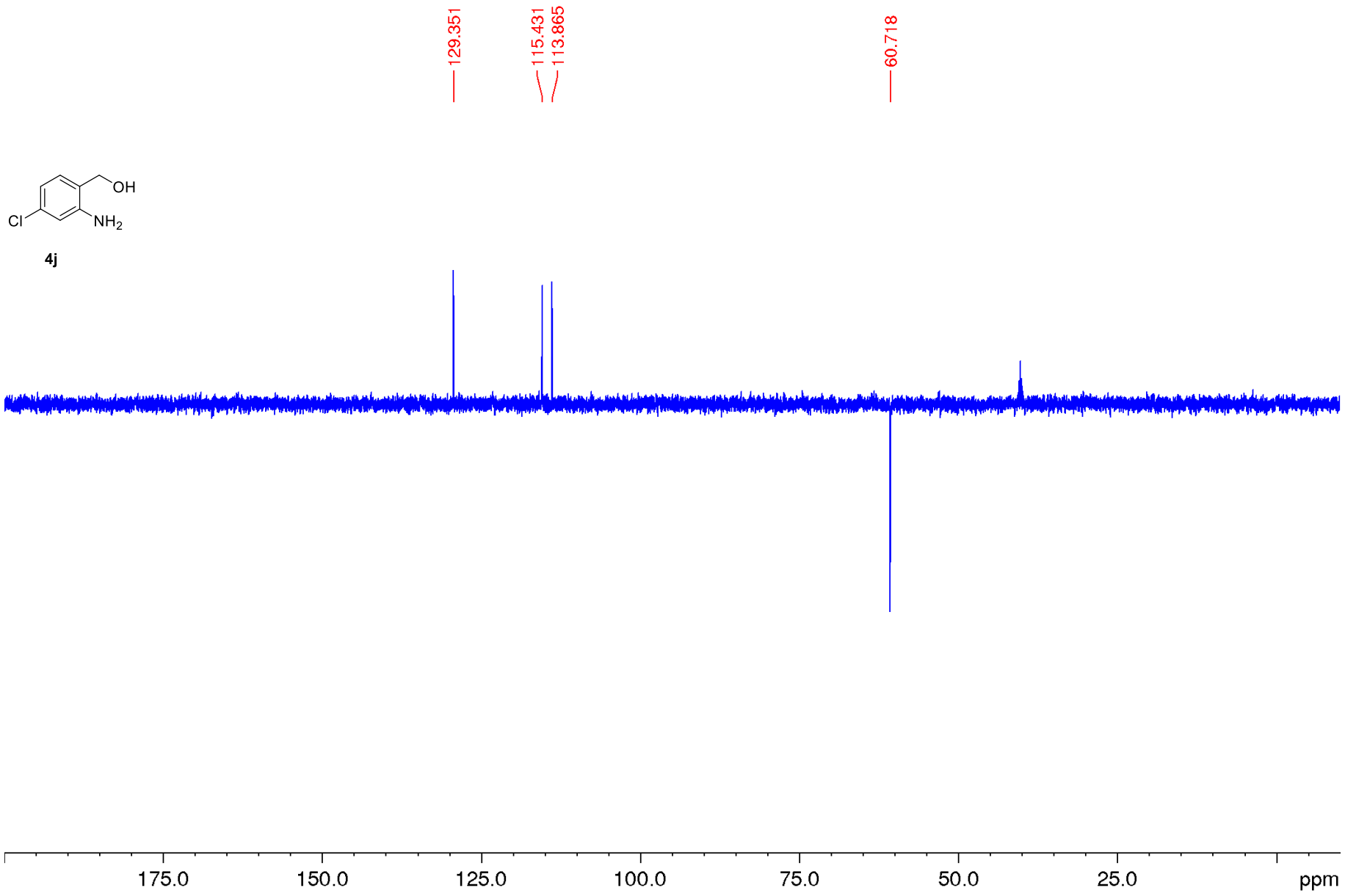
132.238
129.367
124.684
115.444
113.885
60.739
OH
Cl
NH2
4j
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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115.431
113.865
60.718
OH
Cl
NH2
4j
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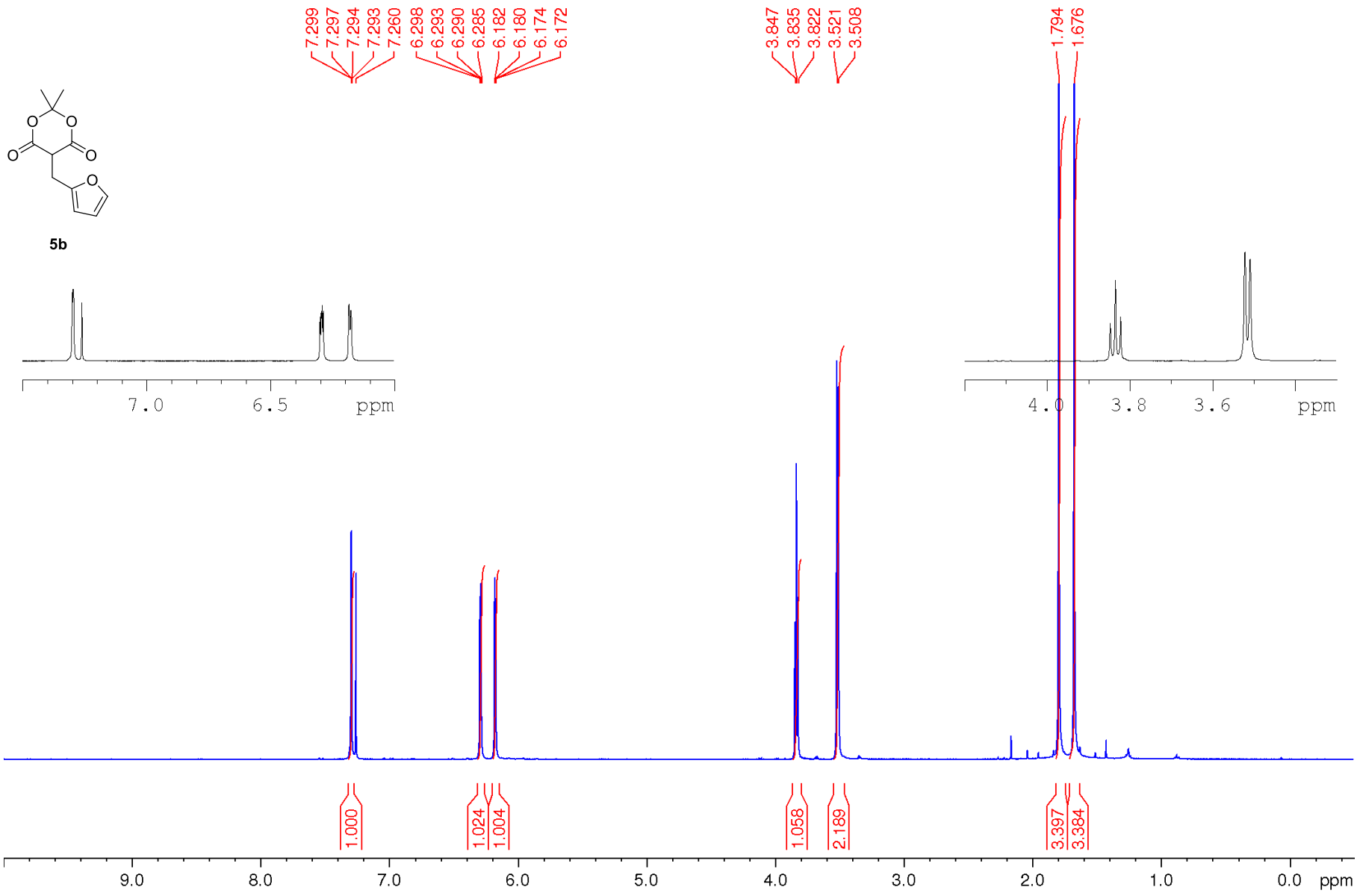
150.0
125.0
100.0
75.0
50.0
25.0
ppm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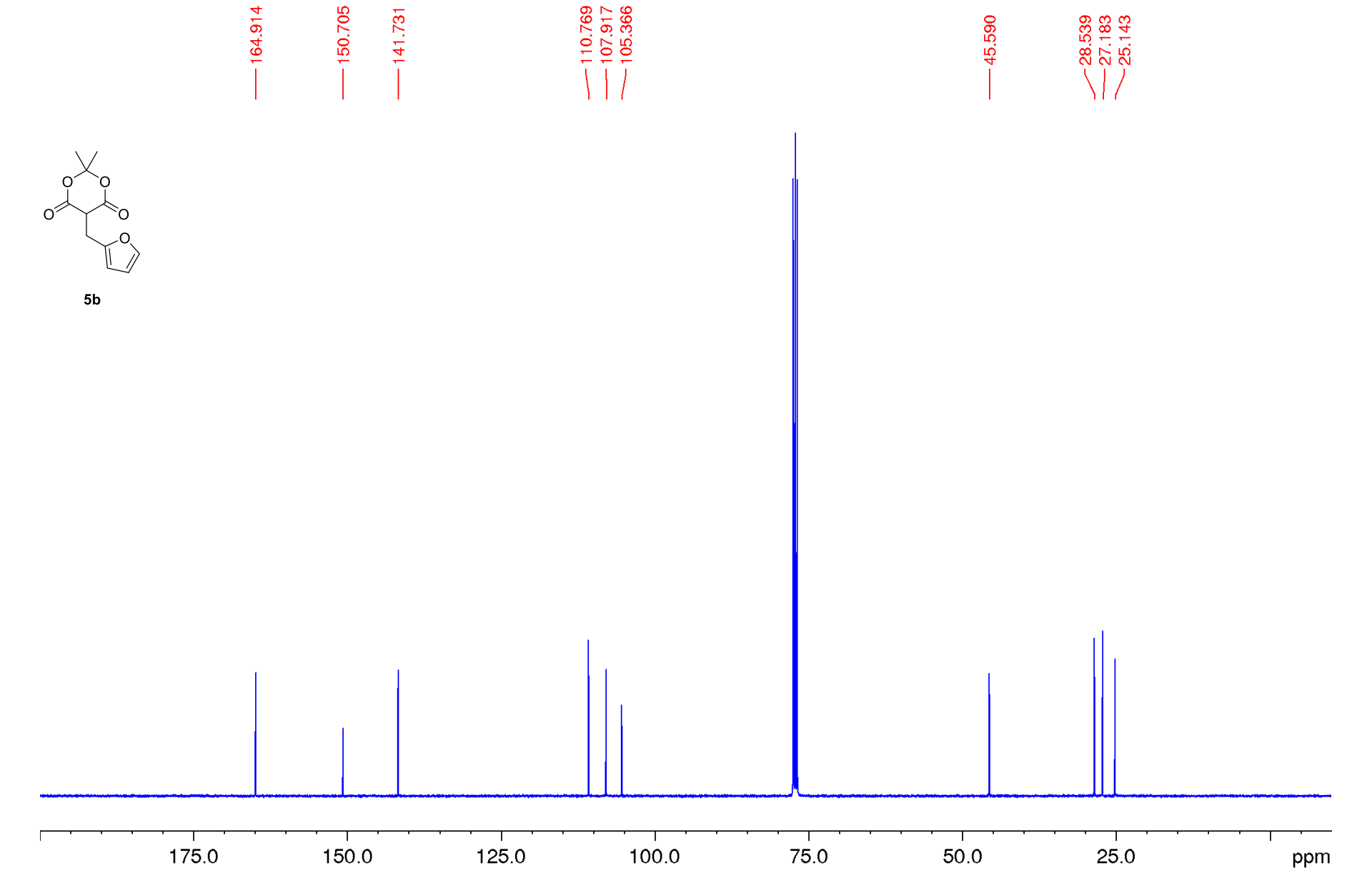
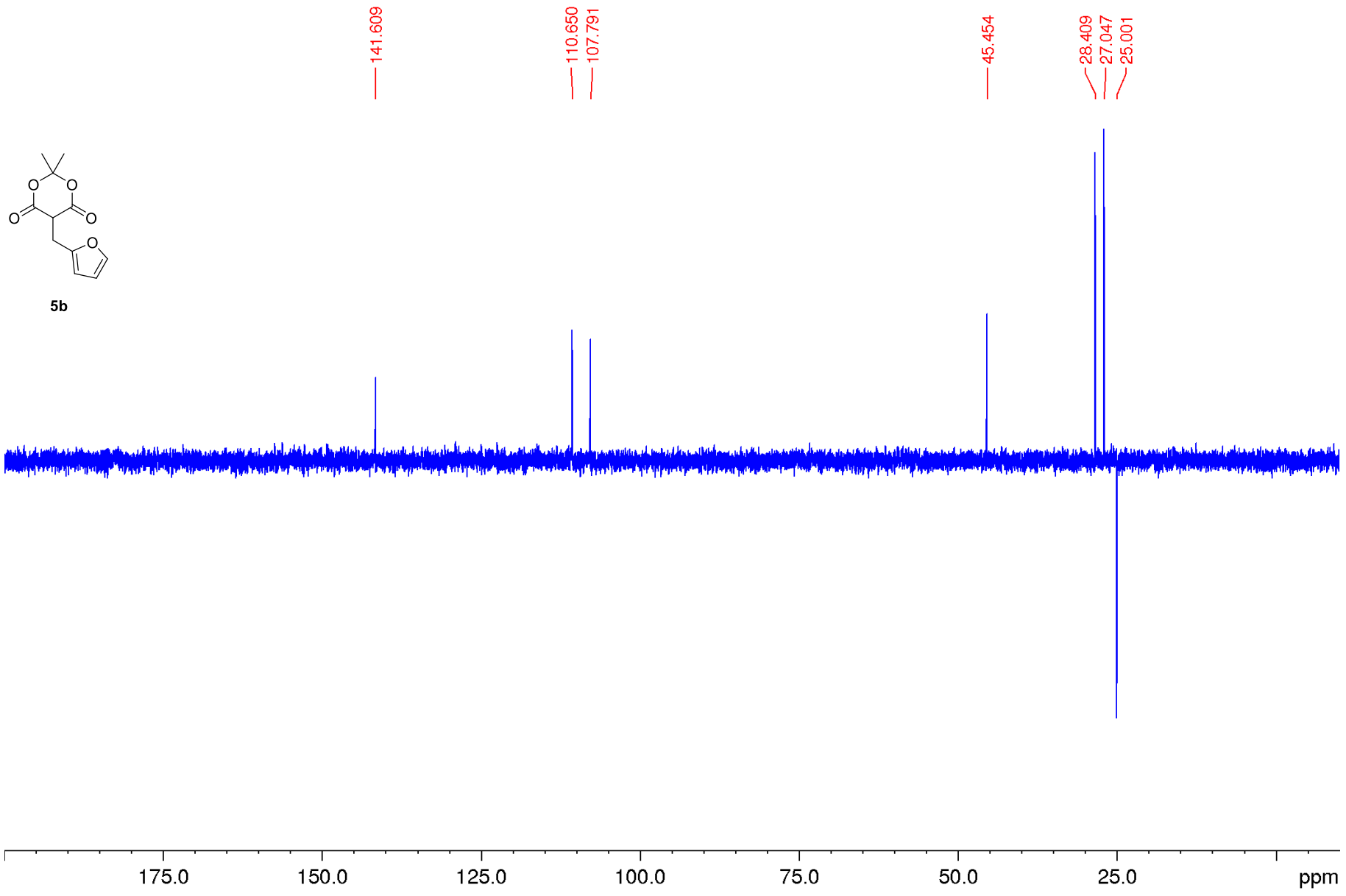
7.297
7.294
7.293
7.260
6.298
6.293
6.290
6.285
6.182
6.180
6.174
6.172
3.847
3.835
3.822
3.521
3.508
1.794
1.676
5b
7.0
6.5
ppm
4.0
3.8
3.6
ppm
1.000
1.024
1.004
1.058
2.189
3.397
3.384
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


164.914
150.705
141.731
110.769
107.917
105.366
45.590
28.539
27.183
25.143
5b
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


141.609
110.650
107.791
45.454
28.409
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25.001
5b
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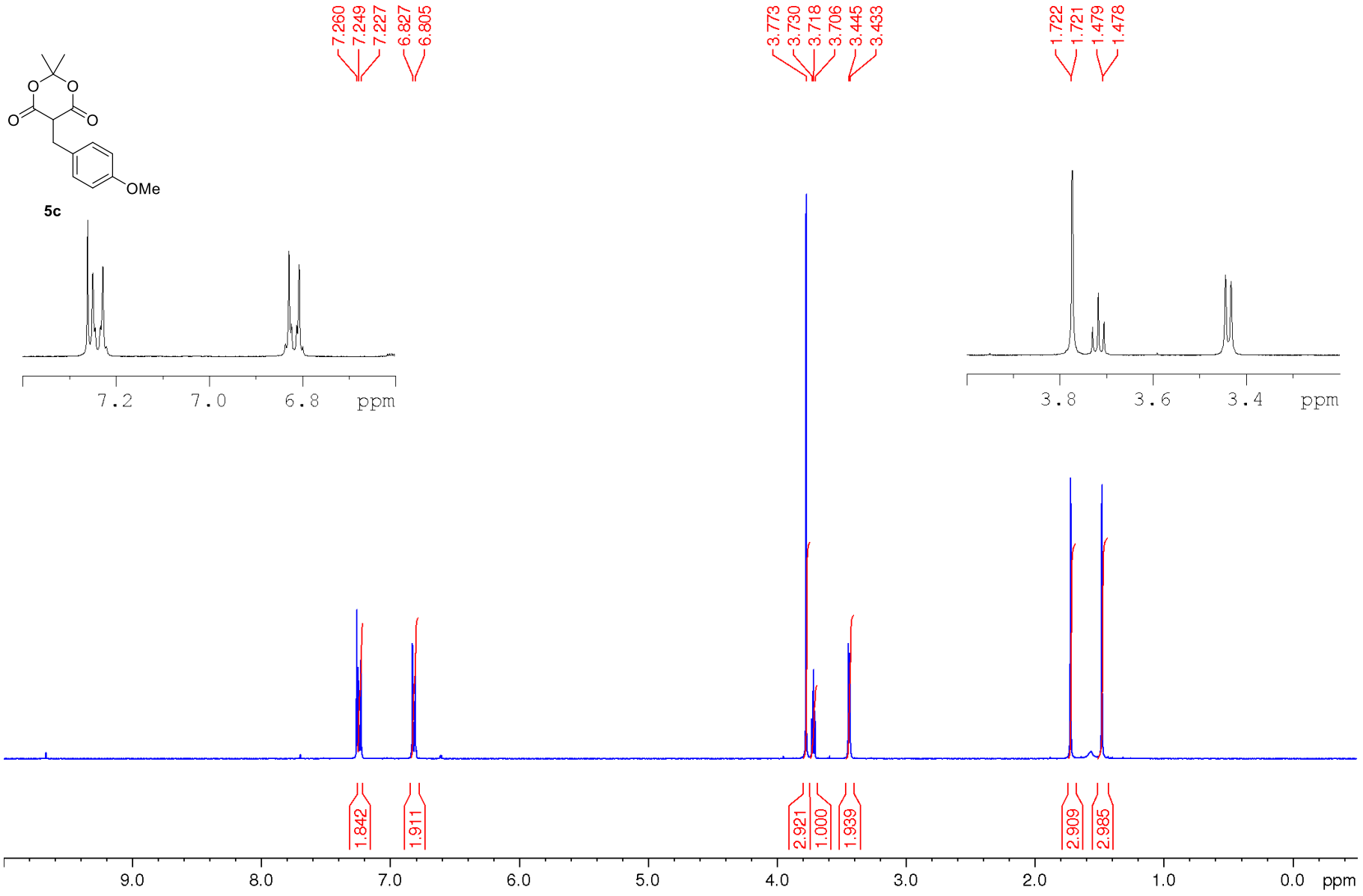
150.0
125.0
100.0
75.0
50.0
25.0
ppm


7.260
7.249
7.227
6.827
6.805
3.773
3.730
3.718
3.706
3.445
3.433
1.722
1.721
1.479
1.478
OMe
5c
7.2
7.0
6.8
ppm
3.8
3.6
3.4
ppm
1.842
1.911
2.921
1.000
1.939
2.909
2.985
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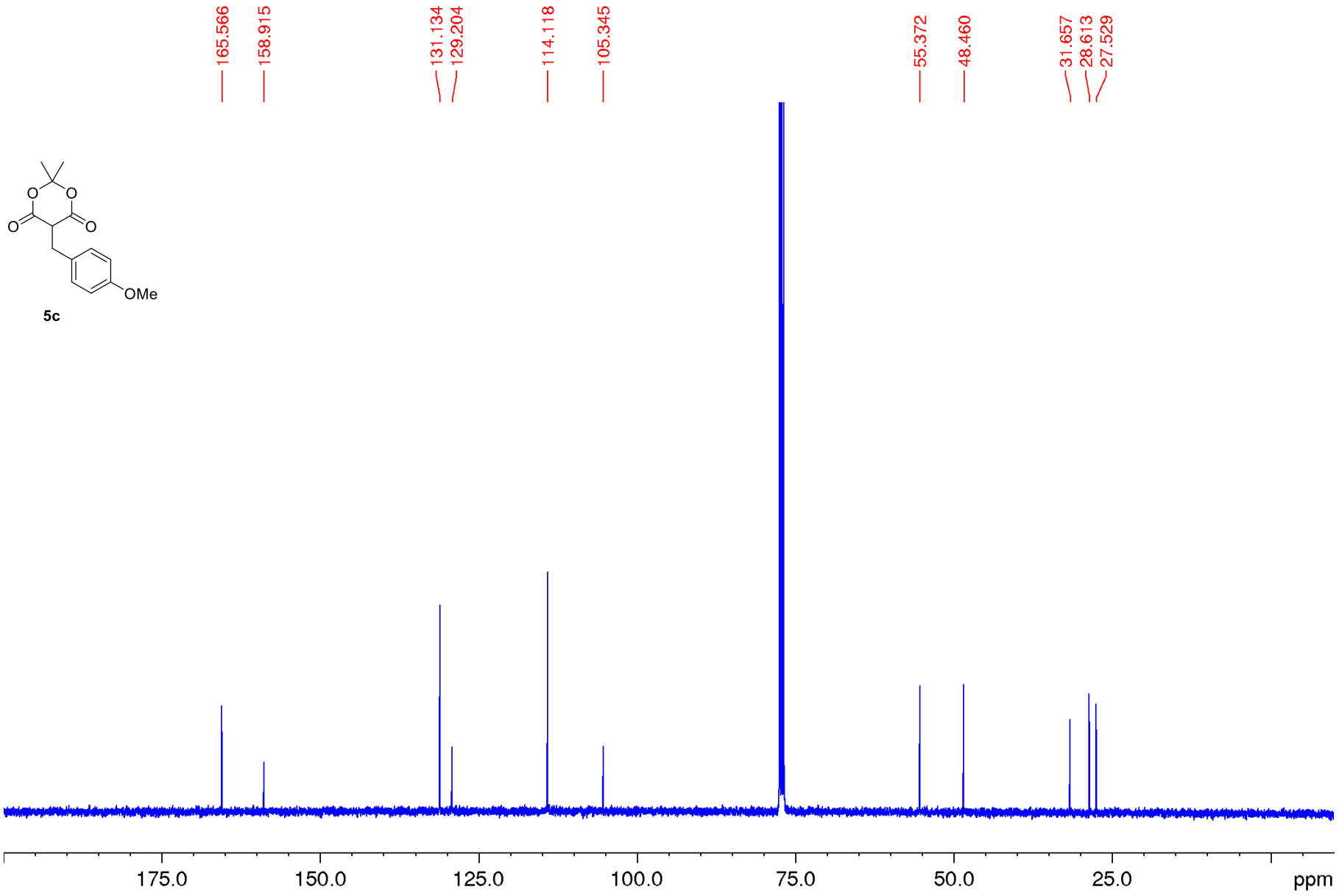
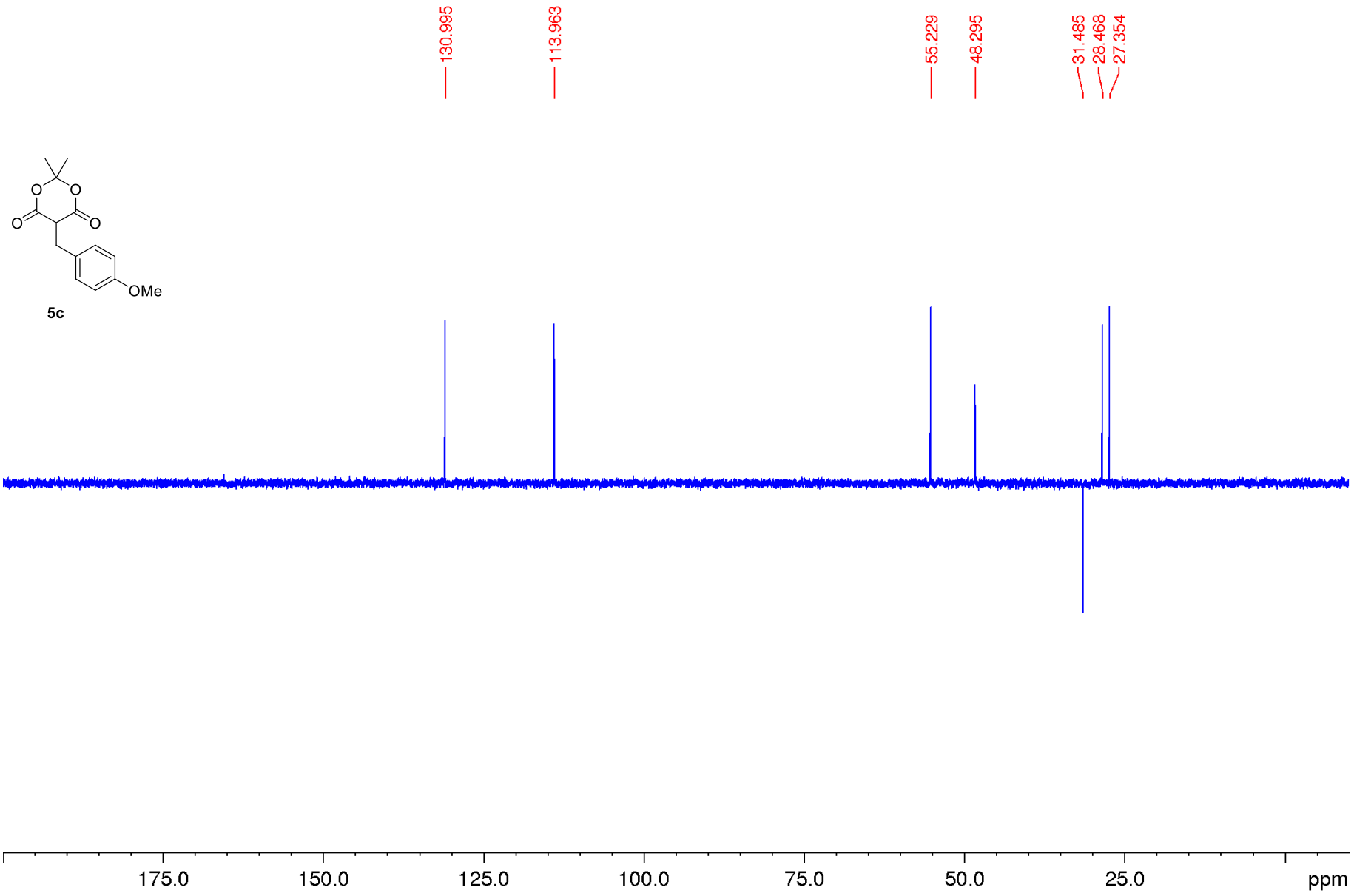
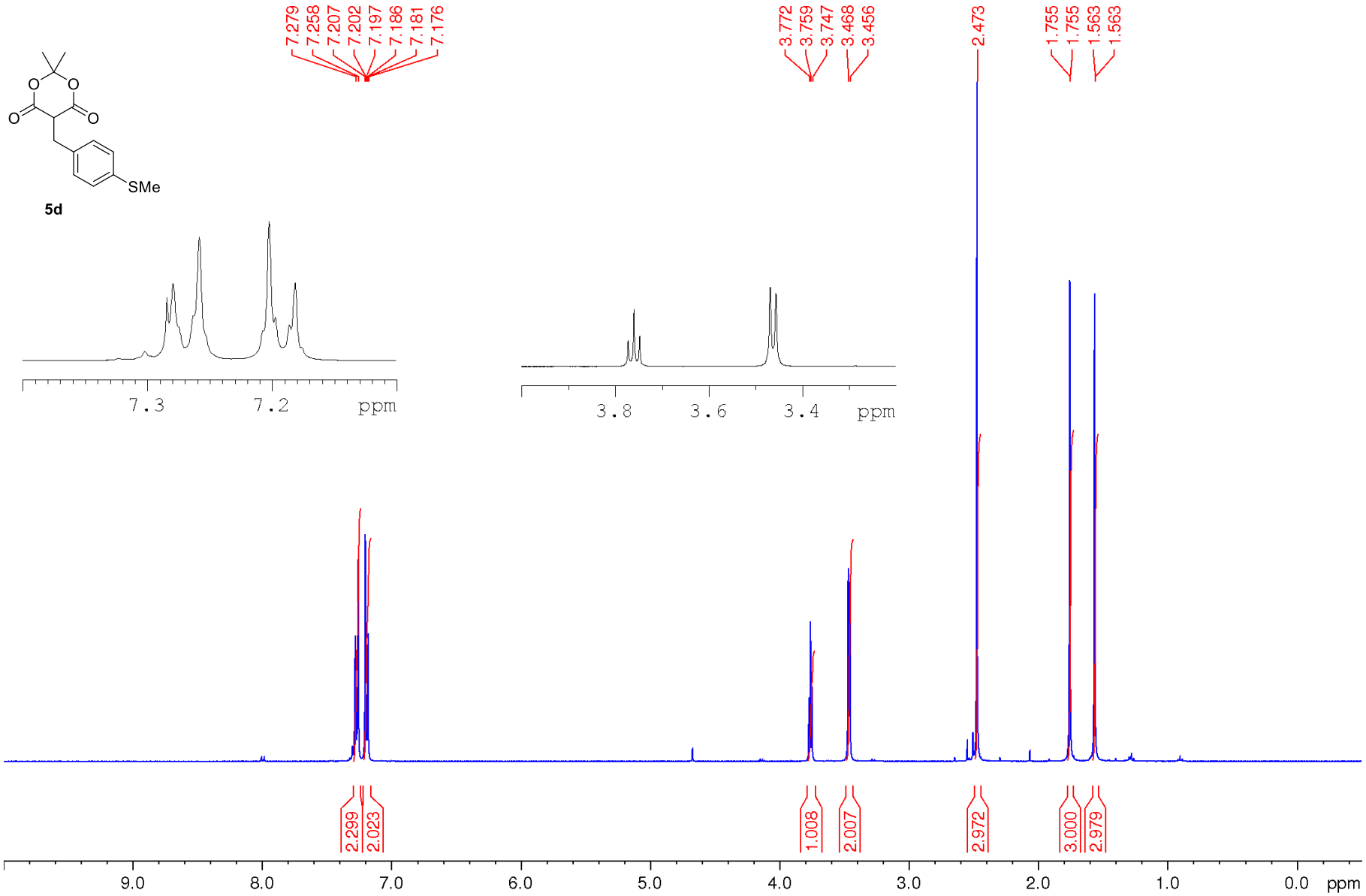
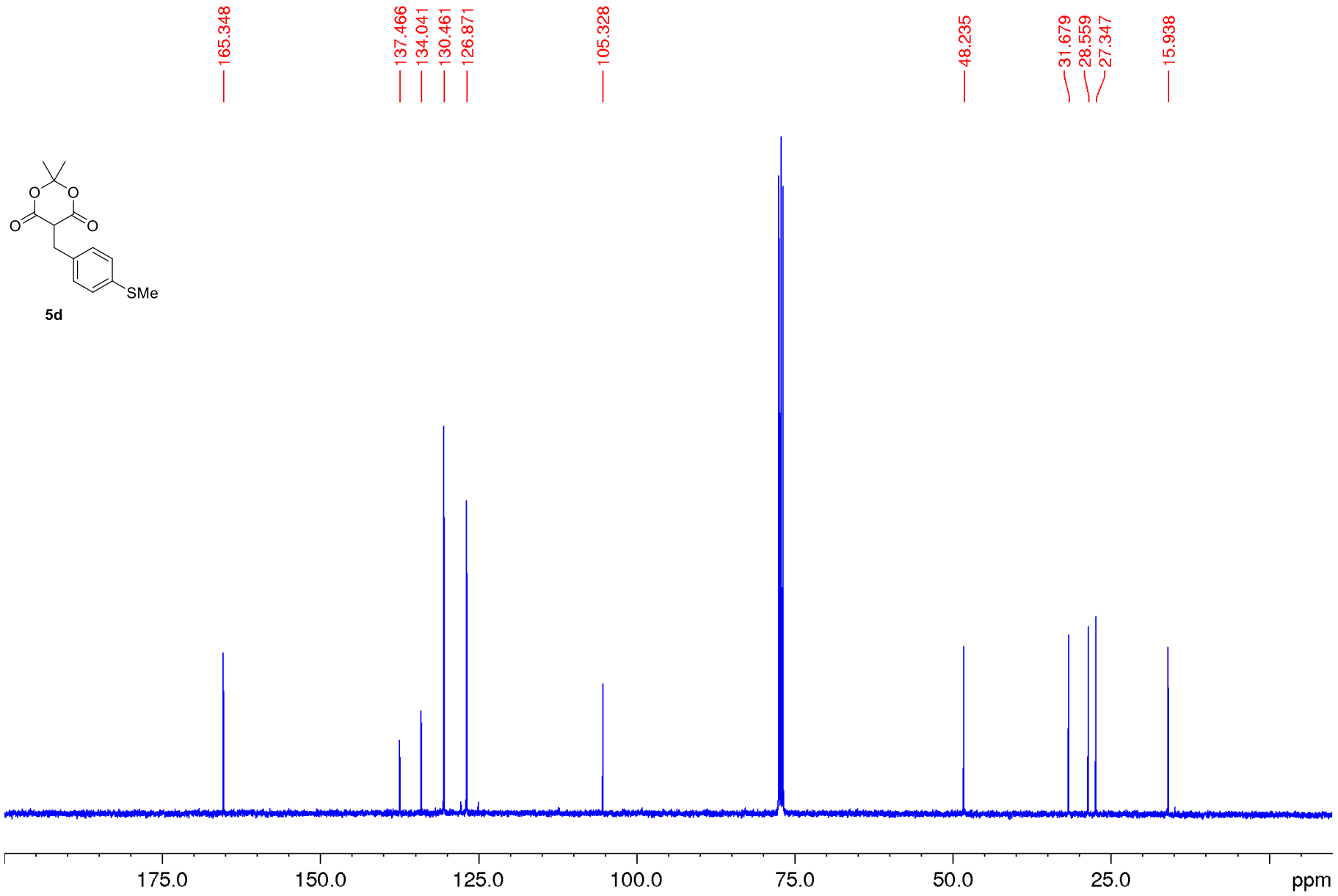
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


165.566
158.915
131.134
129.204
114.118
105.345
55.372
48.460
31.657
28.613
27.529
OMe
5c
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


130.995
113.963
55.229
48.295
31.485
28.468
27.354
OMe
5c
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


7.279
7.258
7.207
7.202
7.197
7.186
7.181
7.176
3.772
3.759
3.747
3.468
3.456
2.473
1.755
1.755
1.563
1.563
SMe
5d
7.3
7.2
ppm
3.8
3.6
3.4
ppm
2.299
2.023
1.008
2.007
2.972
3.000
2.979
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm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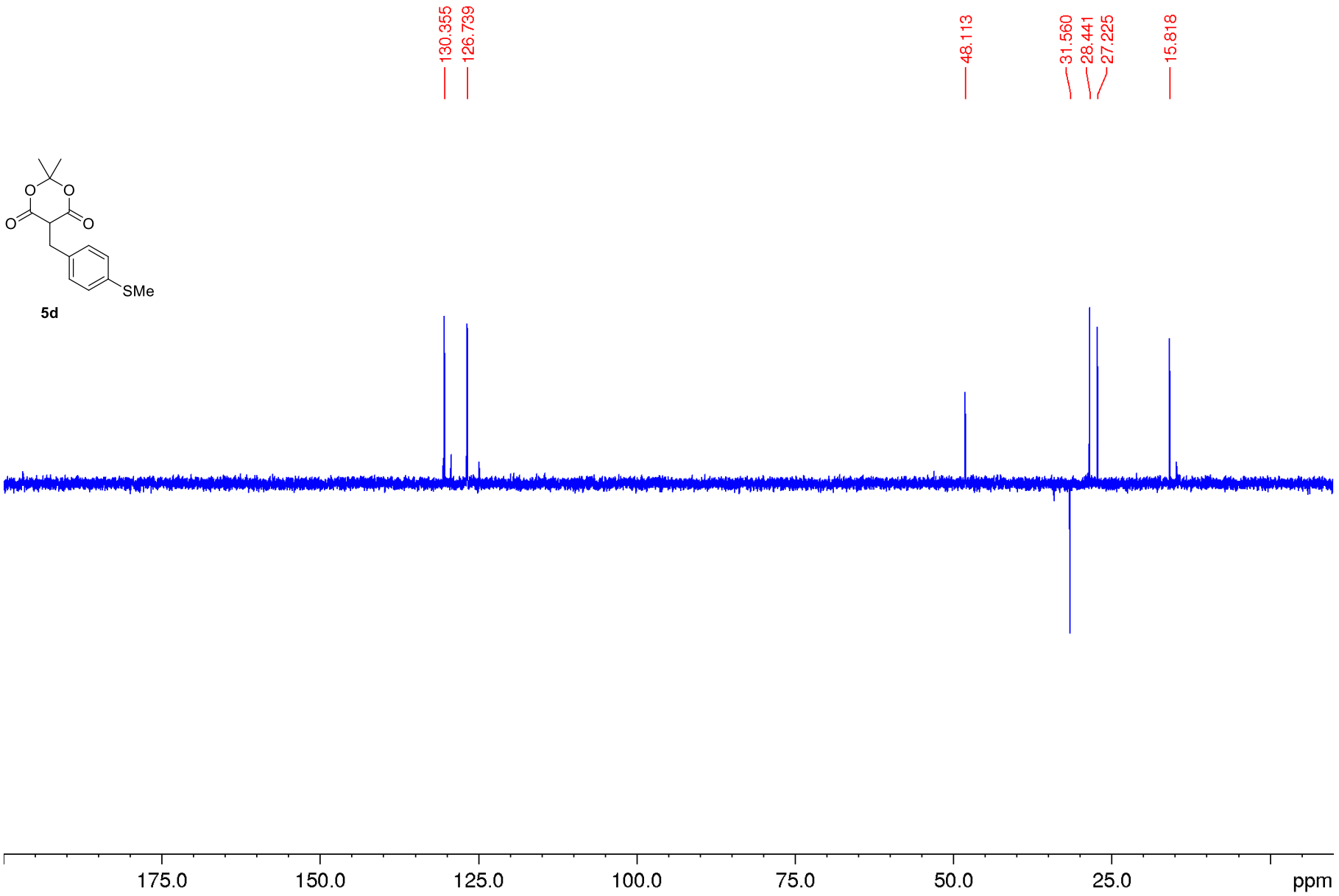
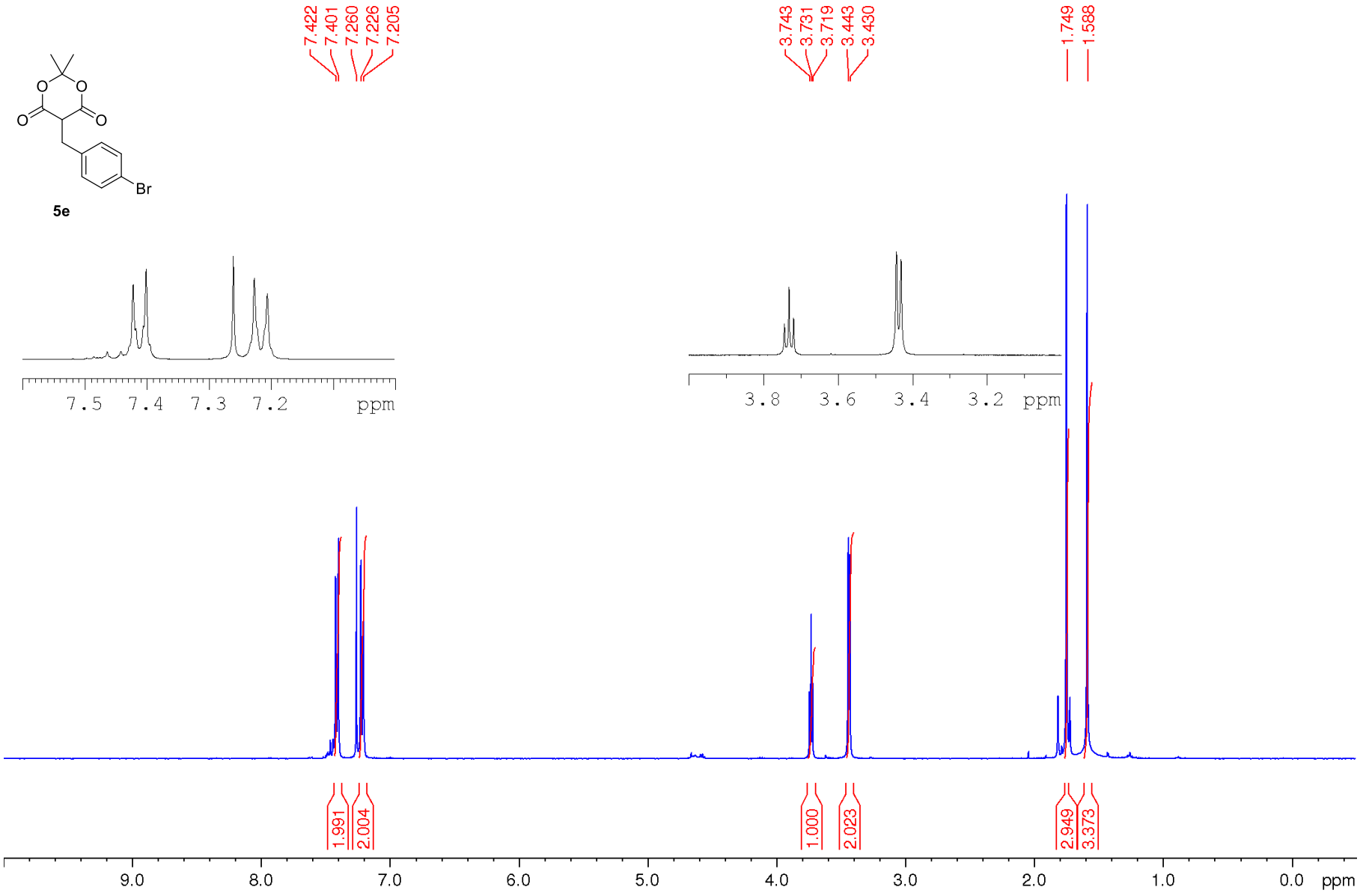
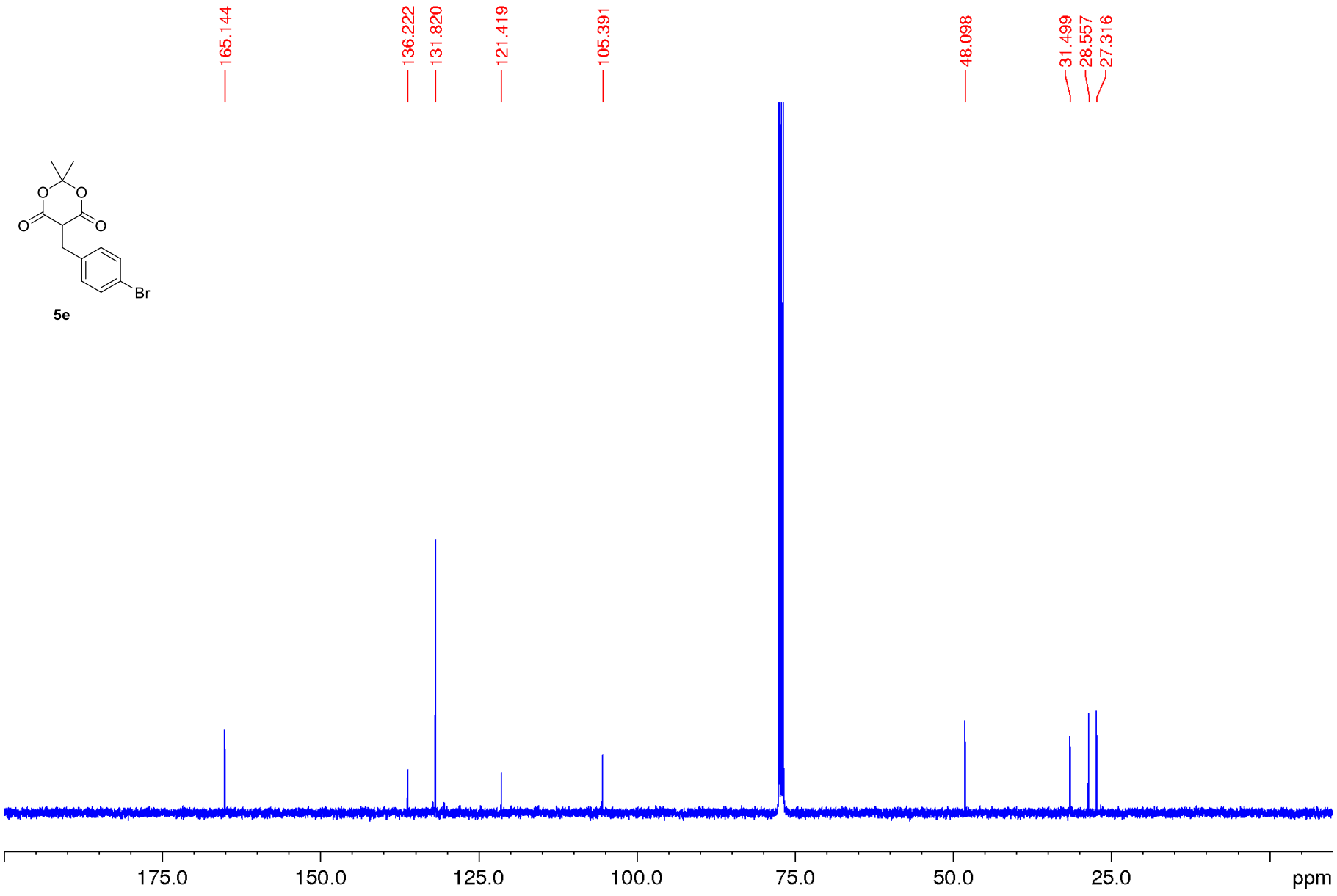
137.466
134.041
130.461
126.871
105.328
48.235
31.679
28.559
27.347
15.938
SMe
5d
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


130.355
126.739
48.113
31.560
28.441
27.225
15.818
O
O
O
O
SMe
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

5d


7.422
7.401
7.260
7.226
7.205
3.743
3.731
3.719
3.443
3.430
1.749
1.588
Br
5e
7.5 7.4 7.3 7.2 ppm
3.8 3.6 3.4 3.2 ppm
1.991
2.004
1.000
2.023
2.949
3.373
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 ppm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136.222
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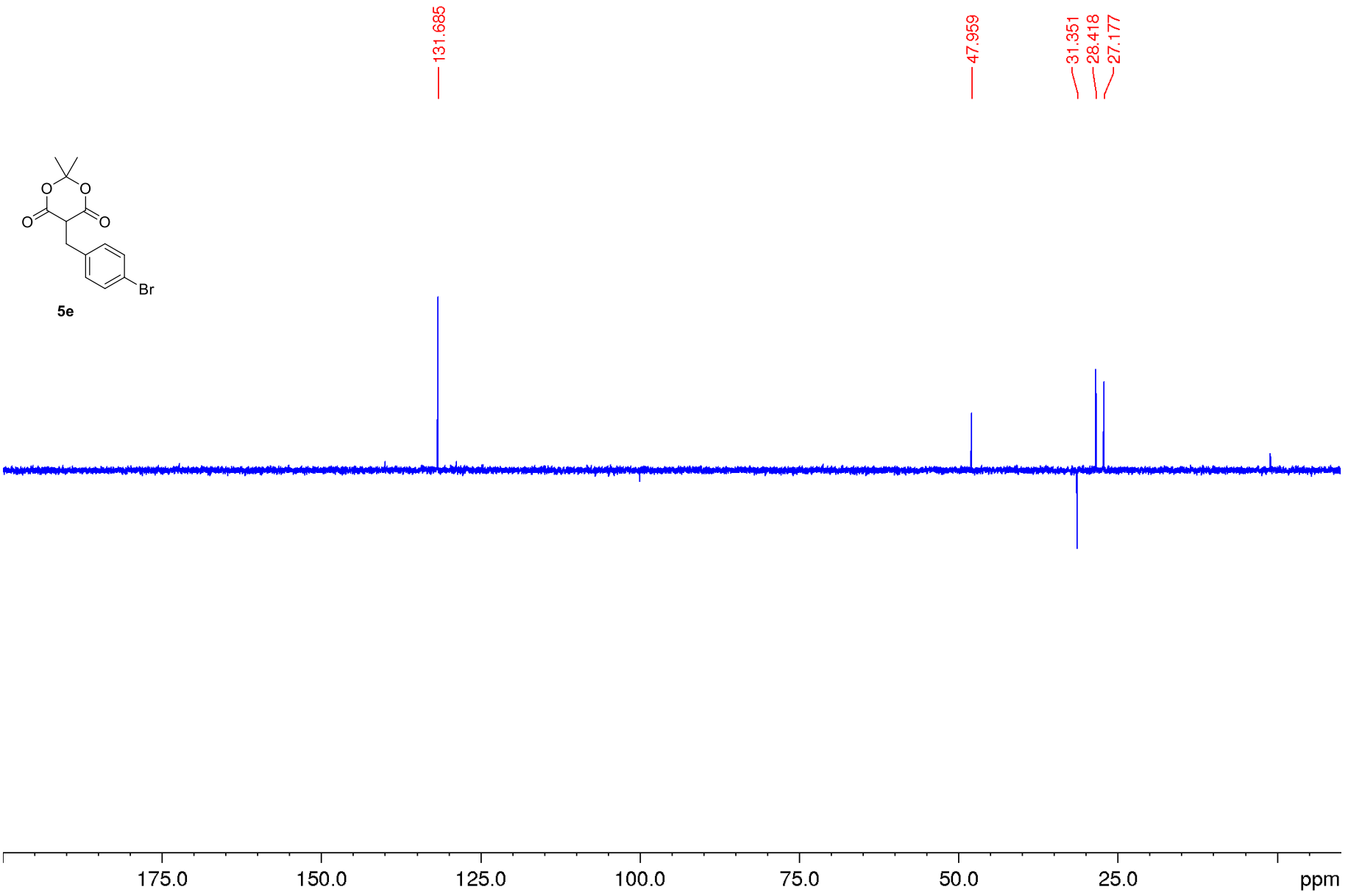
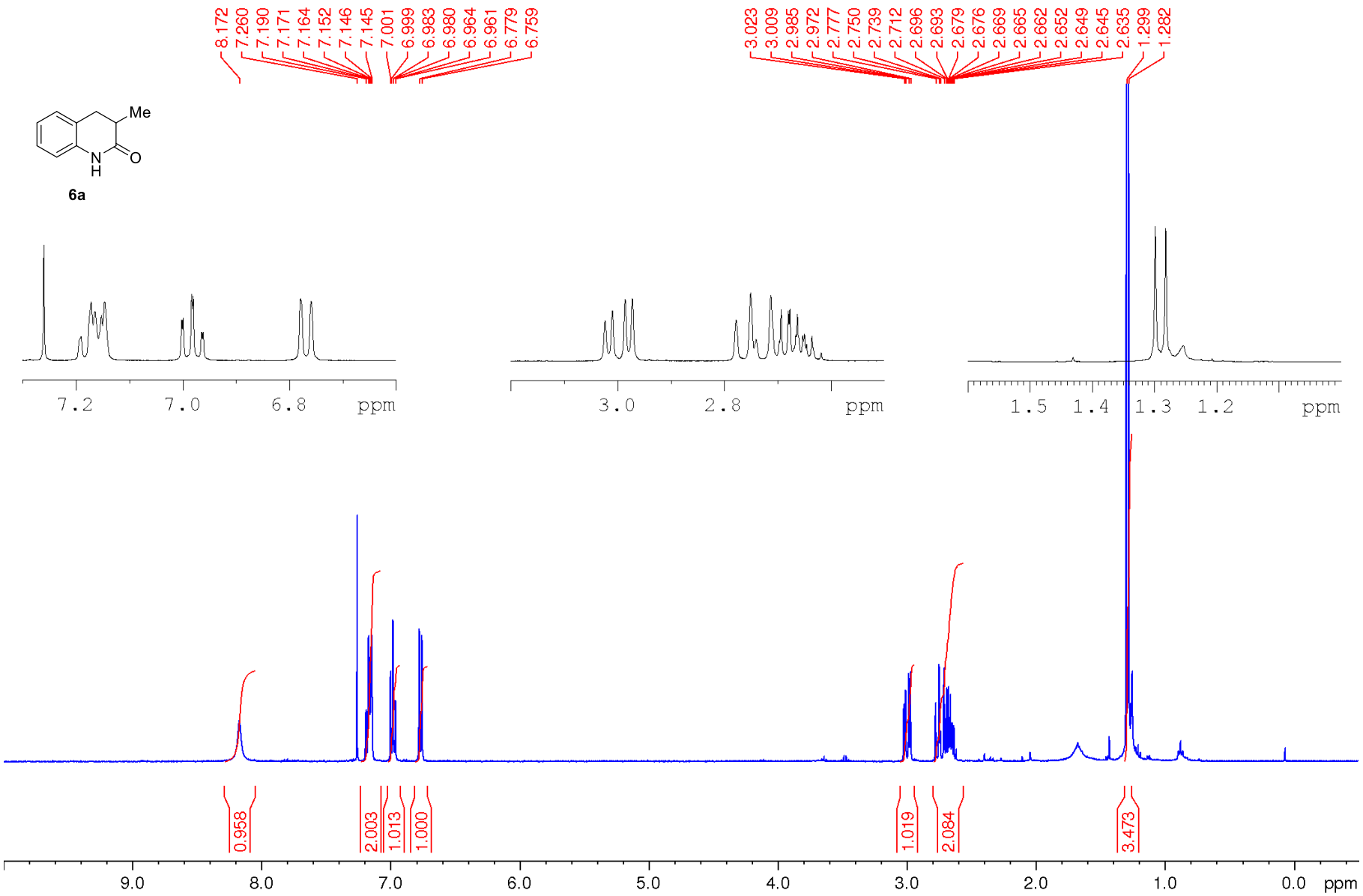
121.419
105.391
48.098
31.499
28.557
27.316
O
O
O
O
Br
5e
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


131.685
47.959
31.351
28.418
27.177
O
O
O
O
Br
5e
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


8.172
7.260
7.190
7.171
7.164
7.152
7.146
7.145
7.001
6.999
6.983
6.980
6.964
6.961
6.779
6.759
3.023
3.009
2.985
2.972
2.777
2.750
2.739
2.712
2.696
2.693
2.679
2.676
2.669
2.665
2.662
2.652
2.649
2.645
2.635
1.299
1.282
Me
N
H
O
6a
7.2
7.0
6.8
ppm
3.0
2.8
ppm
1.5
1.4
1.3
1.2
ppm
0.958
2.003
1.013
1.000
1.019
2.084
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8.0
7.0
6.0
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4.0
3.0
2.0
1.0
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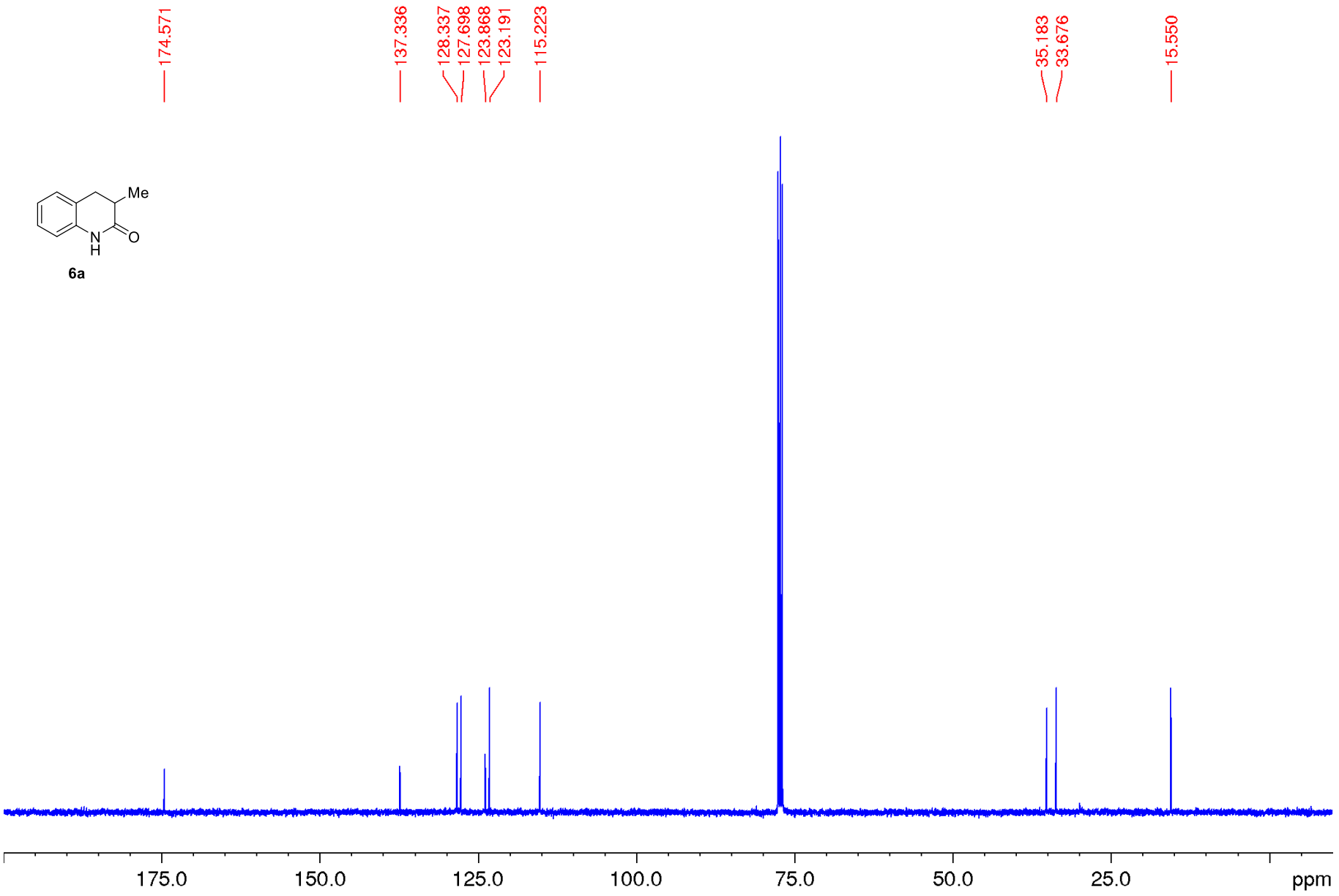
ppm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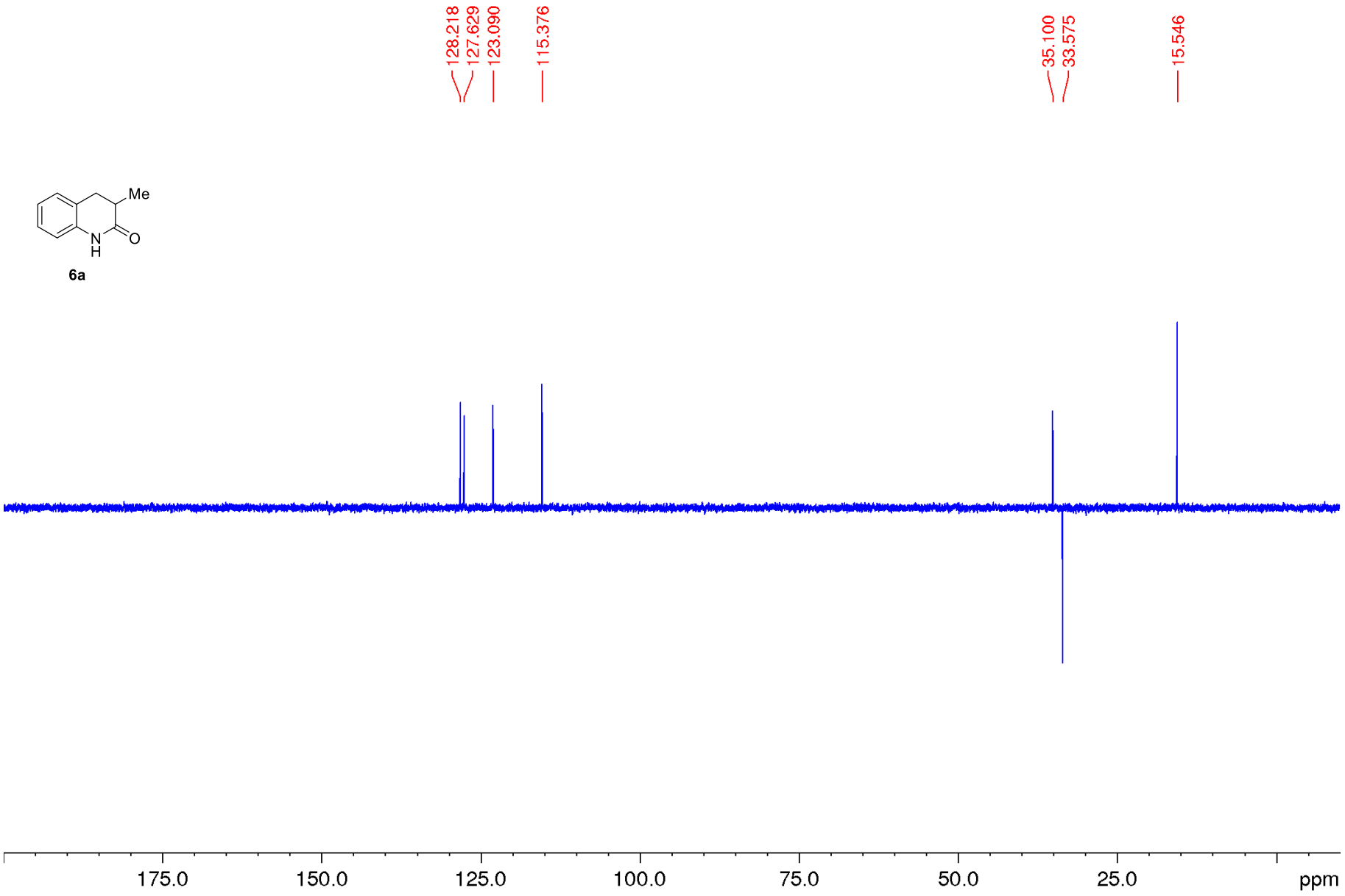
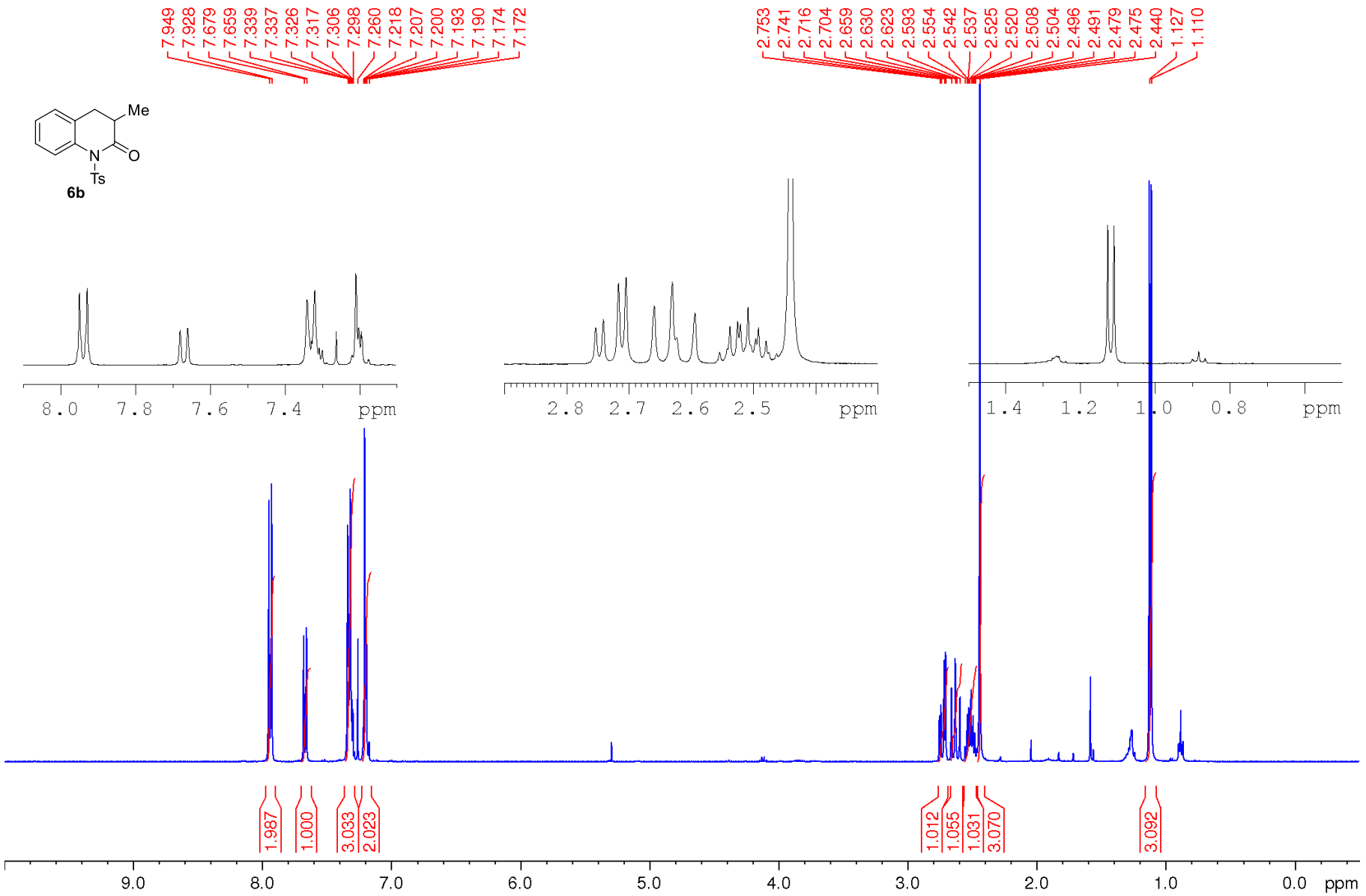
128.337
127.698
123.868
123.191
115.223
35.183
33.676
15.550
Me
N
H
O
6a
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


128.218
127.629
123.090
115.376
35.100
33.575
15.546
Me
N
H
O
6a
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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7.928
7.679
7.659
7.339
7.337
7.326
7.317
7.306
7.298
7.260
7.218
7.207
7.200
7.193
7.190
7.174
7.172
2.753
2.741
2.716
2.704
2.659
2.630
2.623
2.593
2.554
2.542
2.537
2.525
2.520
2.508
2.504
2.496
2.491
2.479
2.475
2.440
1.127
1.110
Me
N
O
Ts
6b
8.0
7.8
7.6
7.4
ppm
2.8
2.7
2.6
2.5
ppm
1.4
1.2
1.0
0.8
ppm
1.987
1.000
3.033
2.023
1.012
1.055
1.031
3.070
3.092
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8.0
7.0
6.0
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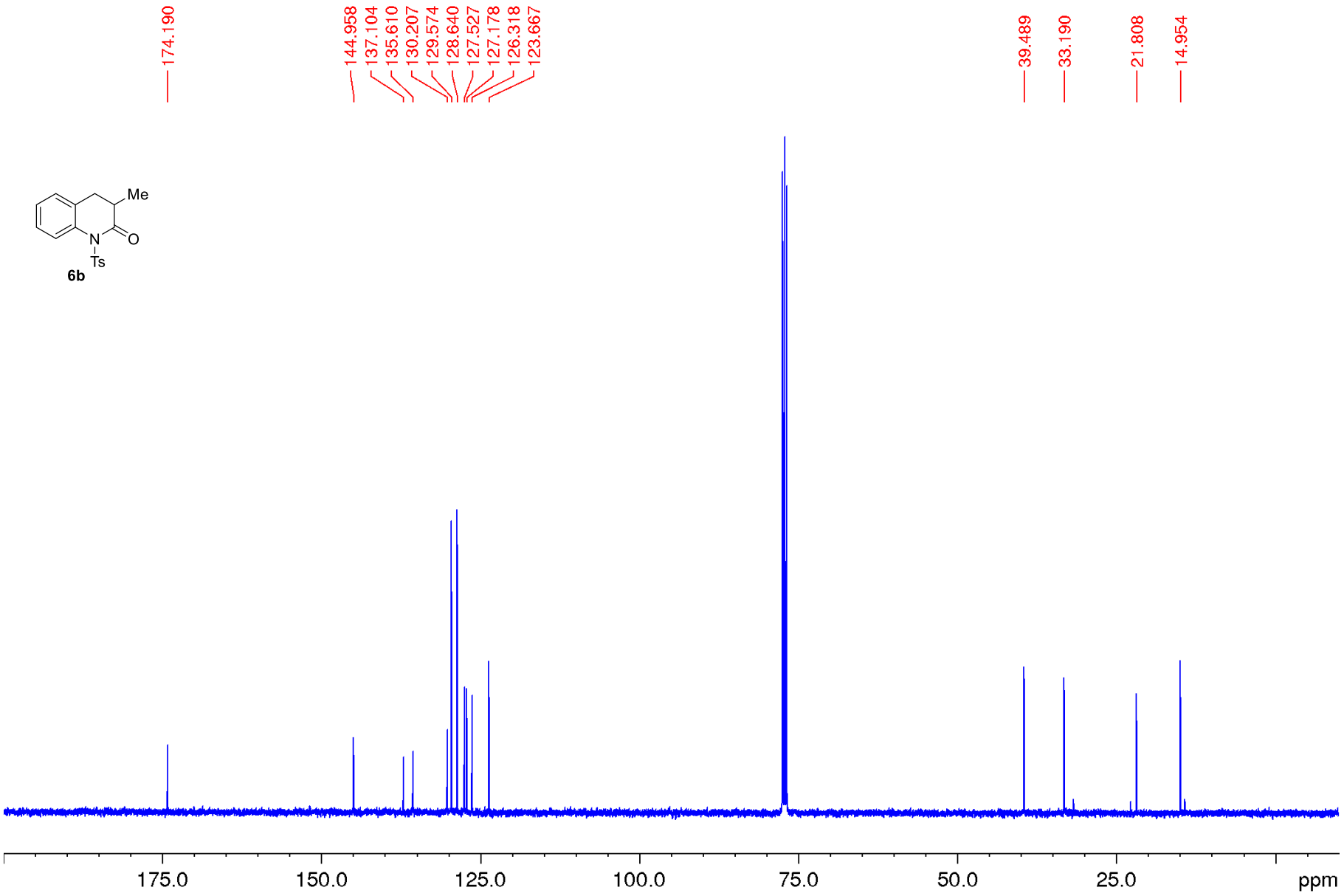
4.0
3.0
2.0
1.0
0.0
ppm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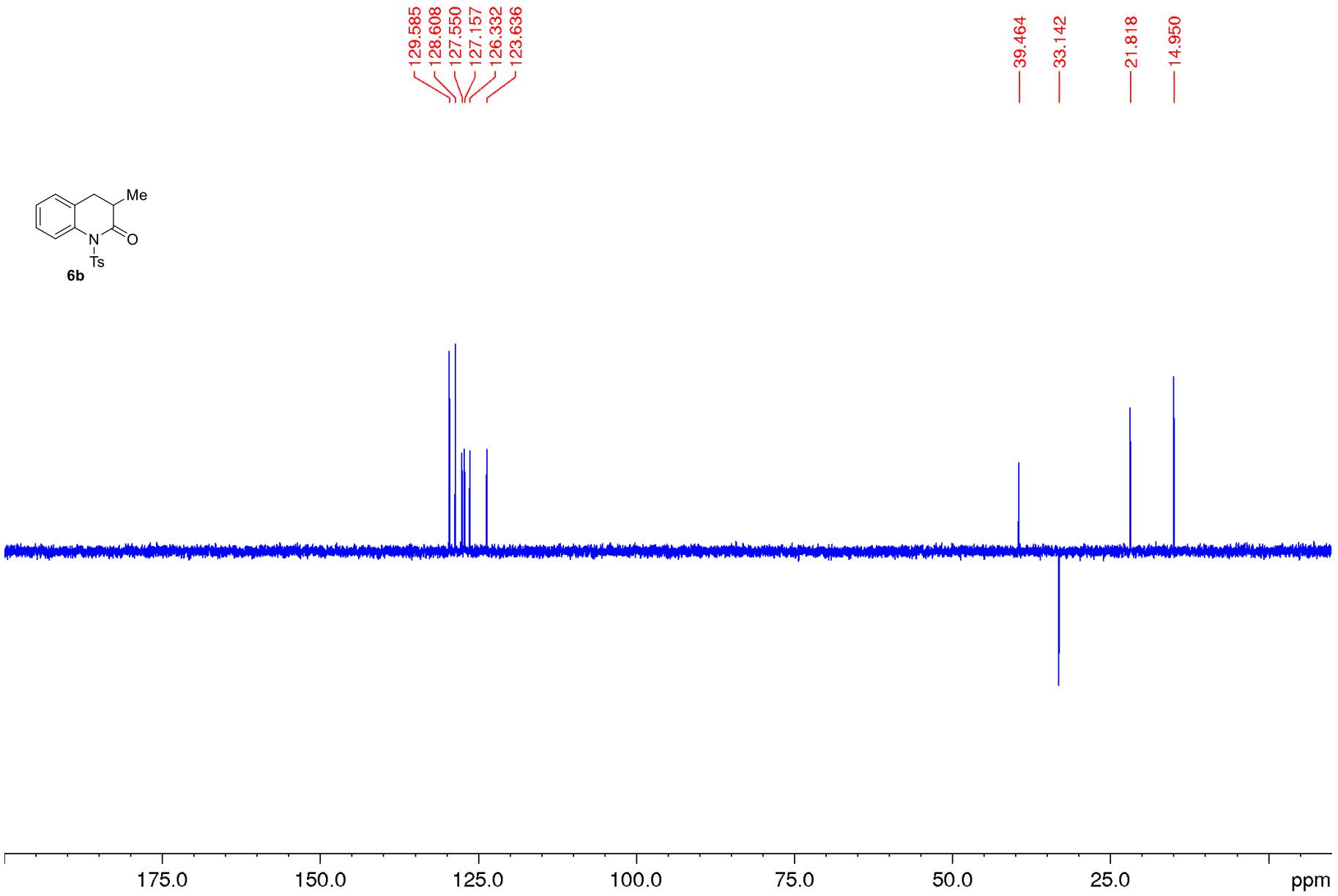
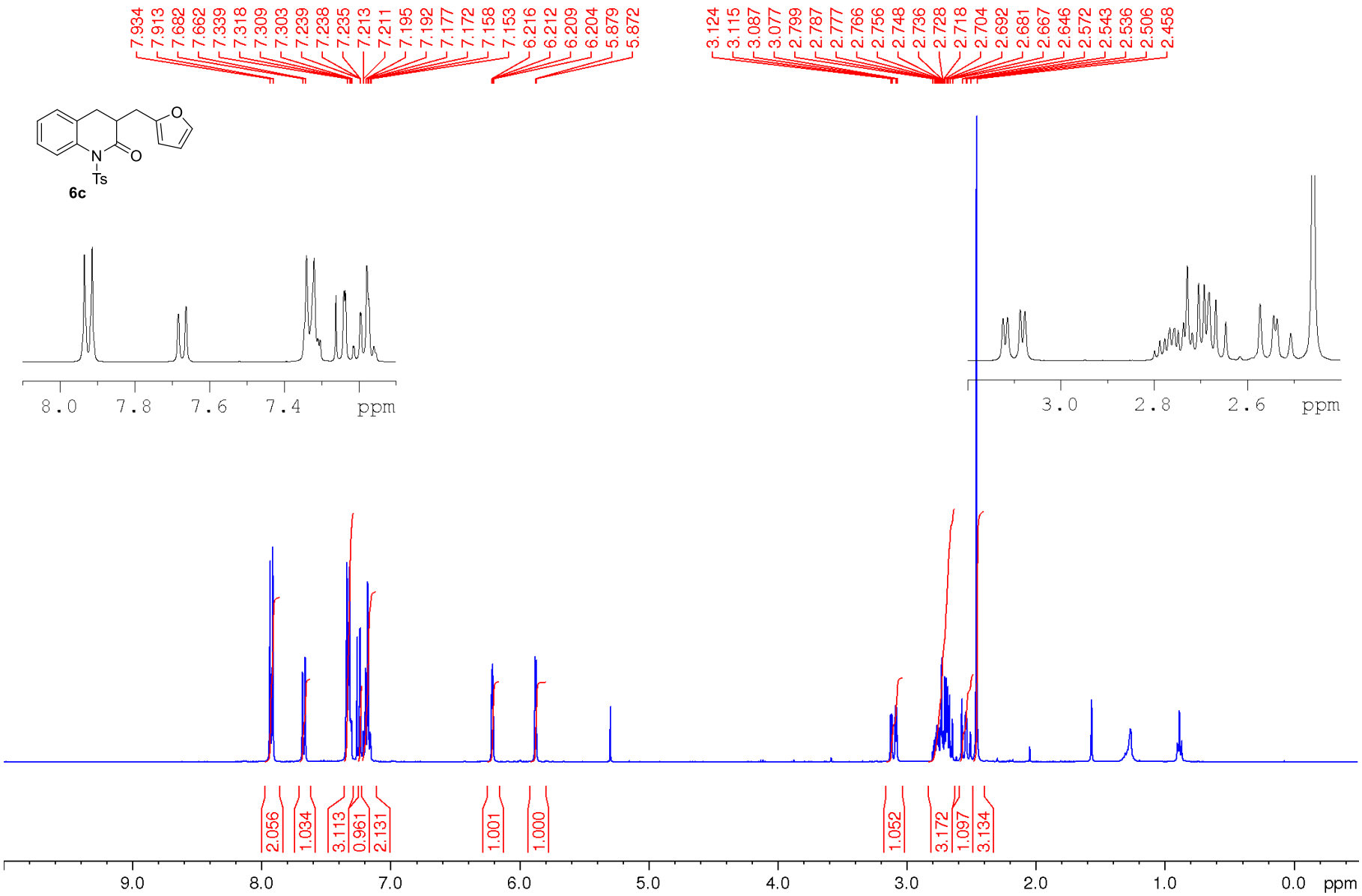
144.958
137.104
135.610
130.207
129.574
128.640
127.527
127.178
126.318
123.667
39.489
33.190
21.808
14.954
Me
N
O
Ts
6b
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


129.585
128.608
127.550
127.157
126.332
123.636
39.464
33.142
21.818
14.950
Me
N
O
Ts
6b
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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7.913
7.682
7.662
7.339
7.318
7.309
7.303
7.239
7.238
7.235
7.213
7.211
7.195
7.192
7.177
7.172
7.158
7.153
6.216
6.212
6.209
6.204
5.879
5.872
3.124
3.115
3.087
3.077
2.799
2.787
2.777
2.766
2.756
2.748
2.736
2.728
2.718
2.704
2.692
2.681
2.667
2.646
2.572
2.543
2.536
2.506
2.458
O
N
O
Ts
6c
8.0
7.8
7.6
7.4
ppm
3.0
2.8
2.6
ppm
2.056
1.034
3.113
0.961
2.131
1.001
1.000
1.052
3.172
1.097
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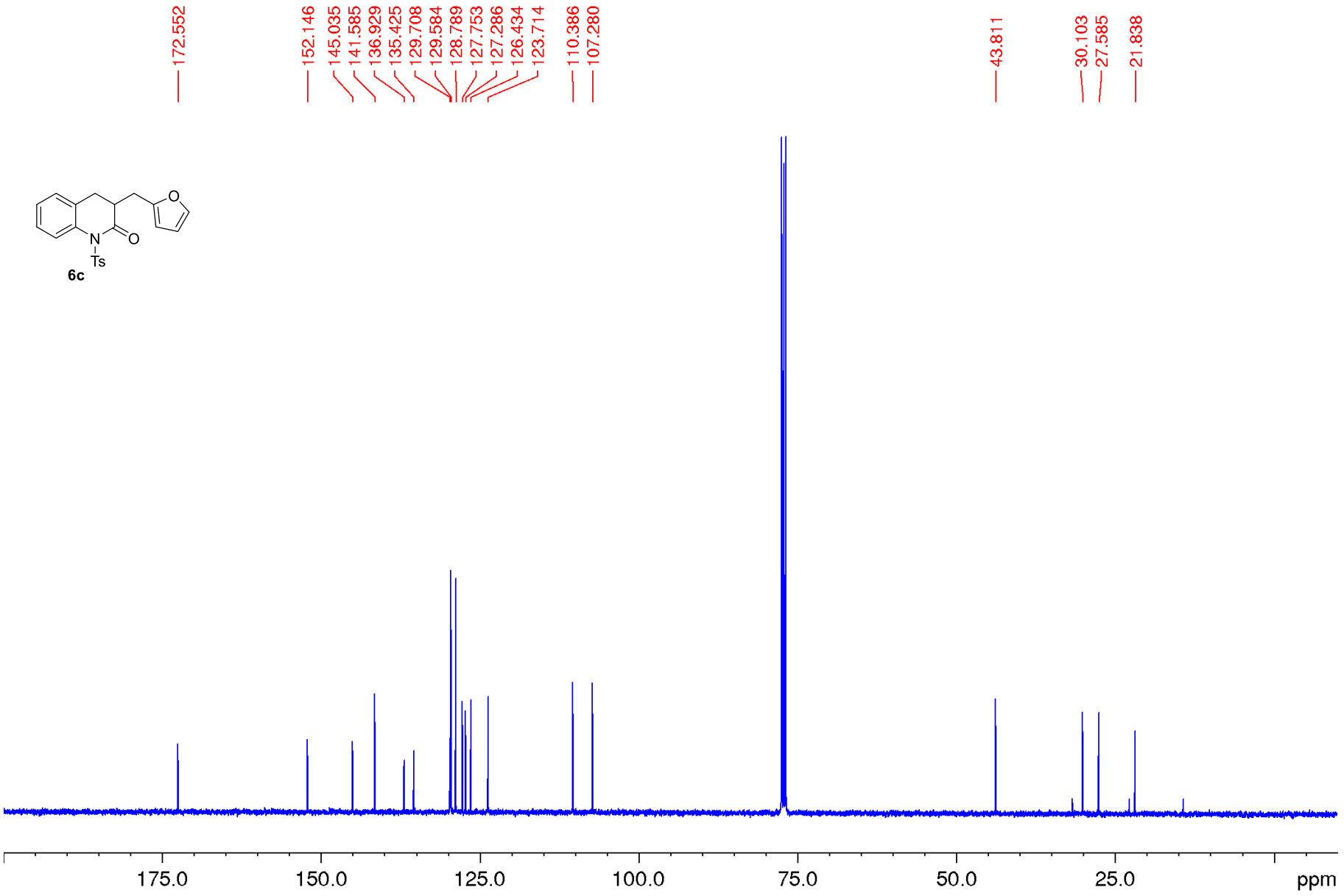
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm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145.035
141.585
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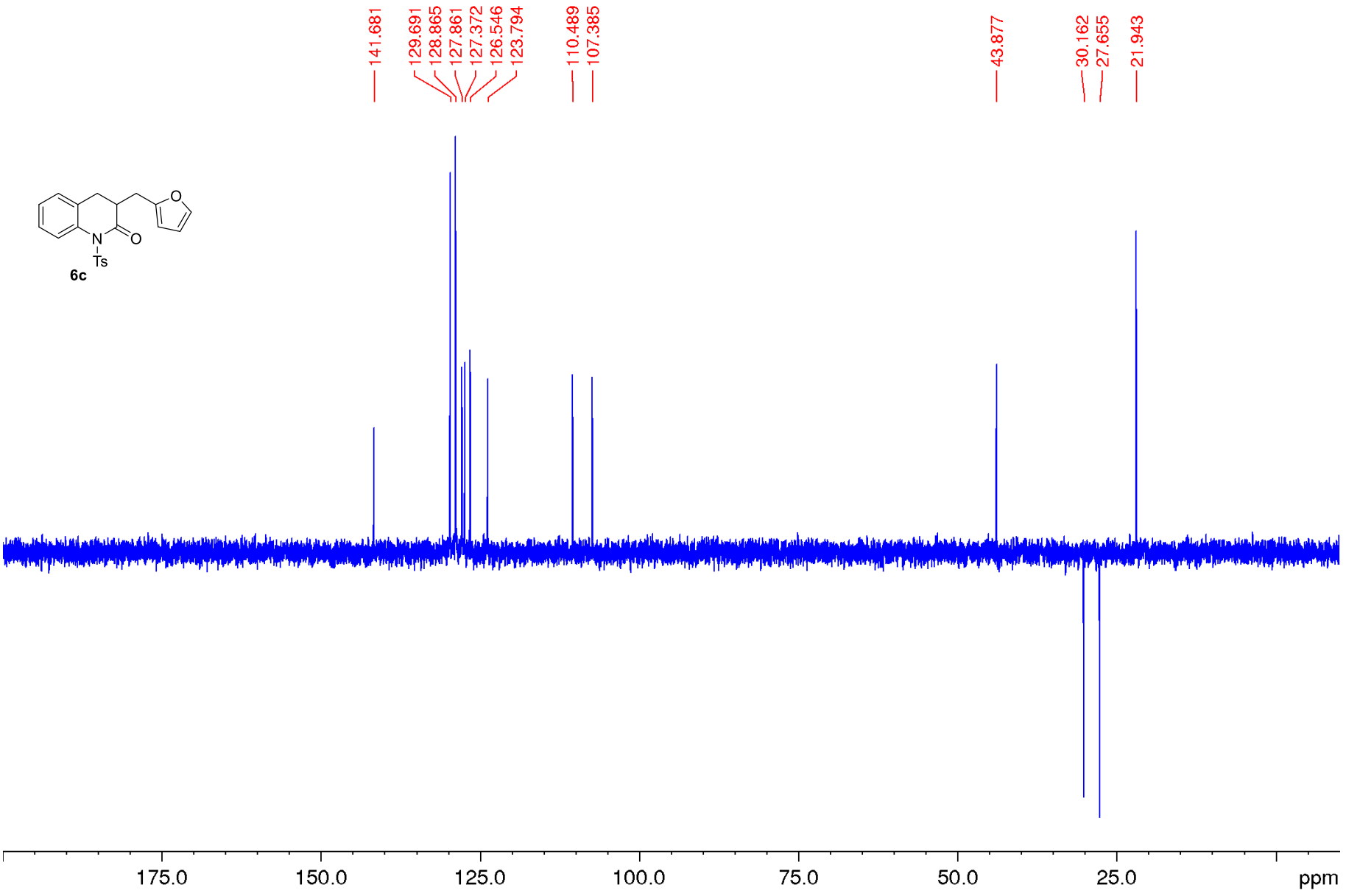
129.584
128.789
127.753
127.286
126.434
123.714
110.386
107.280
43.811
30.103
27.585
21.838
O
N
O
Ts
6c
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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127.372
126.546
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110.489
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43.877
30.162
27.655
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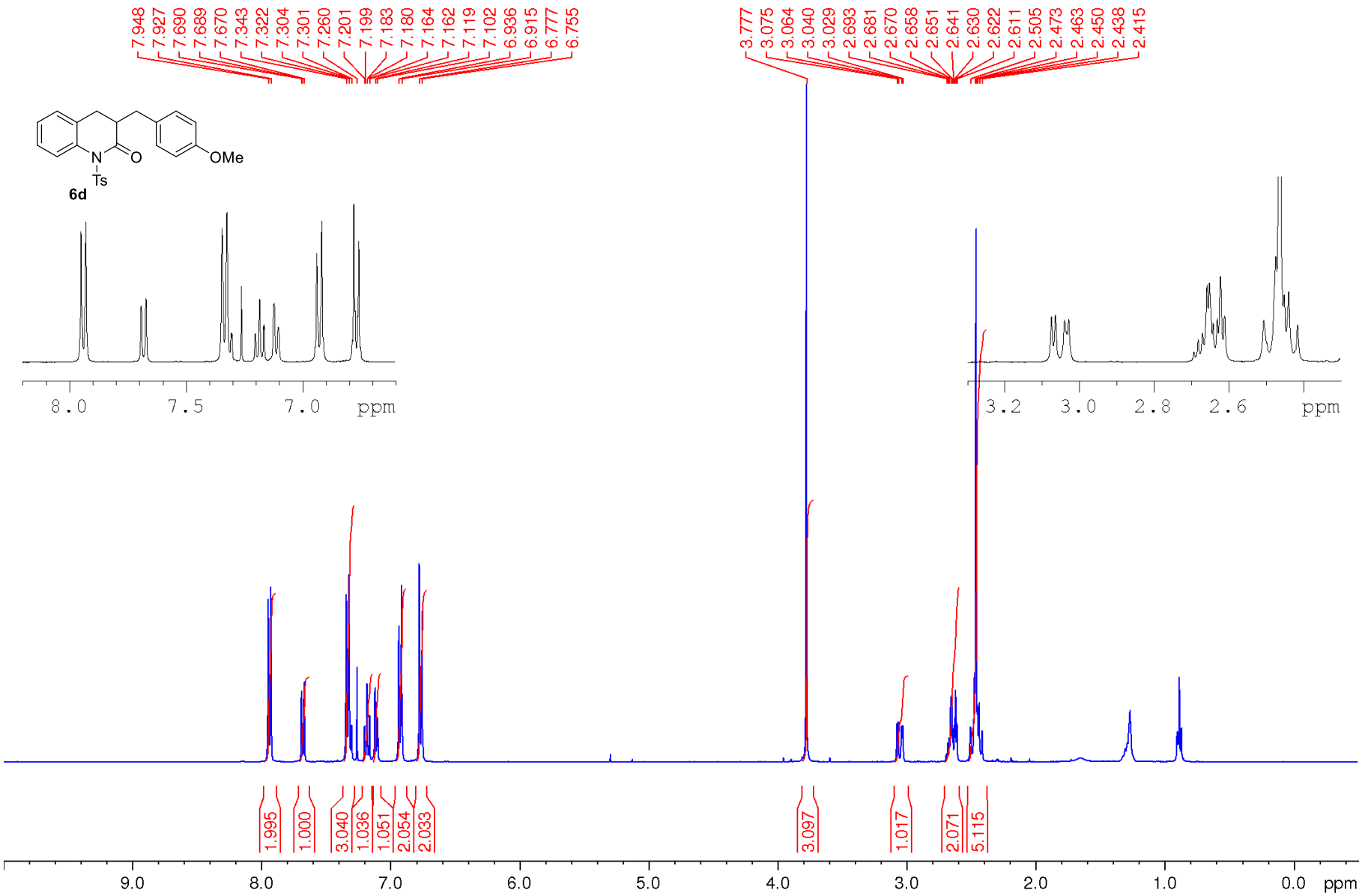
O
Ts
6c
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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7.689
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7.343
7.322
7.304
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7.260
7.201
7.199
7.183
7.180
7.164
7.162
7.119
7.102
6.936
6.915
6.777
6.755
3.777
3.075
3.064
3.040
3.029
2.693
2.681
2.670
2.658
2.651
2.641
2.630
2.622
2.611
2.505
2.473
2.463
2.450
2.438
2.415
N
O
OMe
Ts
6d
8.0
7.5
7.0
ppm
3.2
3.0
2.8
2.6
ppm
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1.000
3.040
1.036
1.051
2.054
2.033
3.097
1.017
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3.0
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1.0
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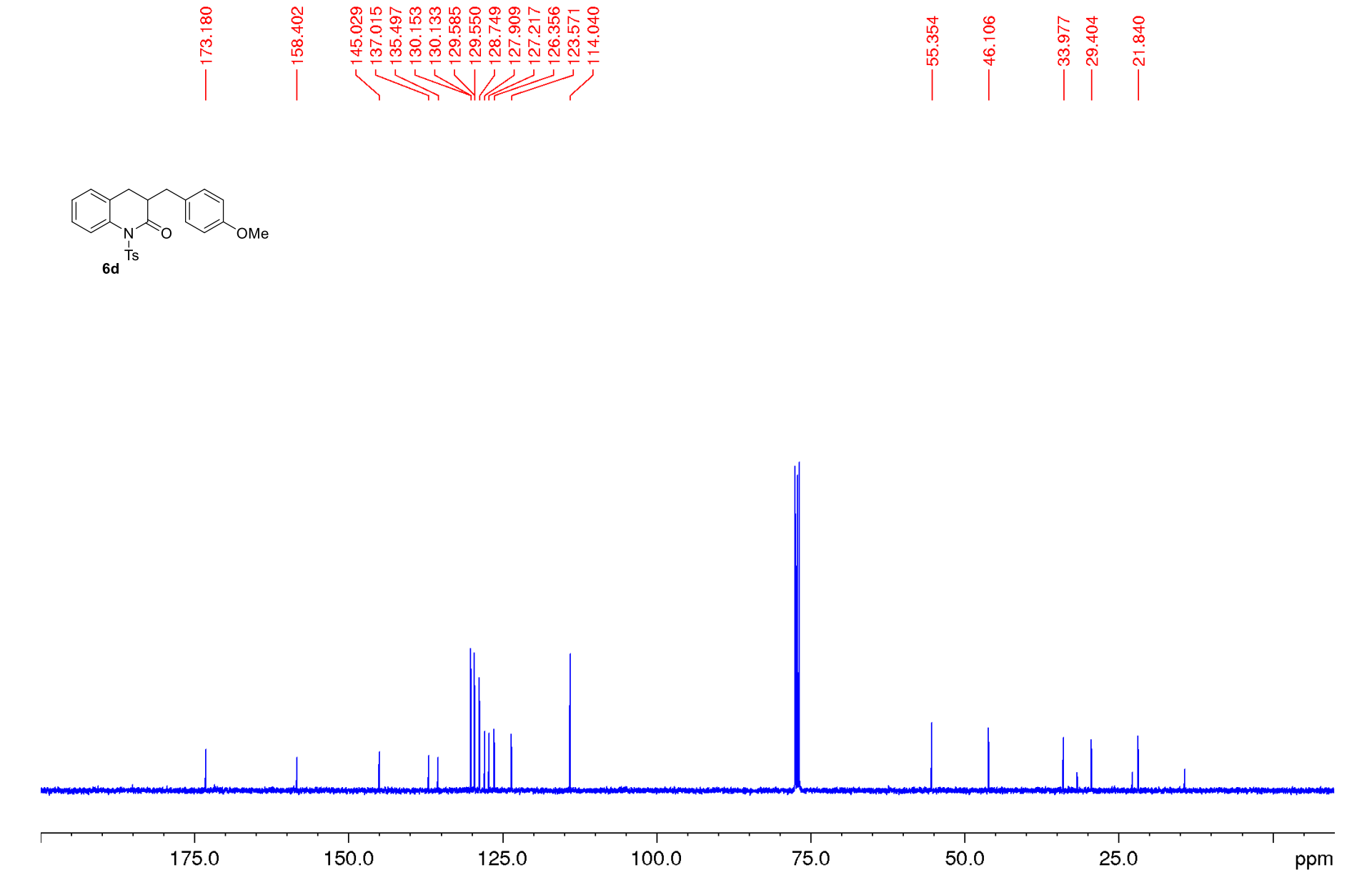
ppm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129.585
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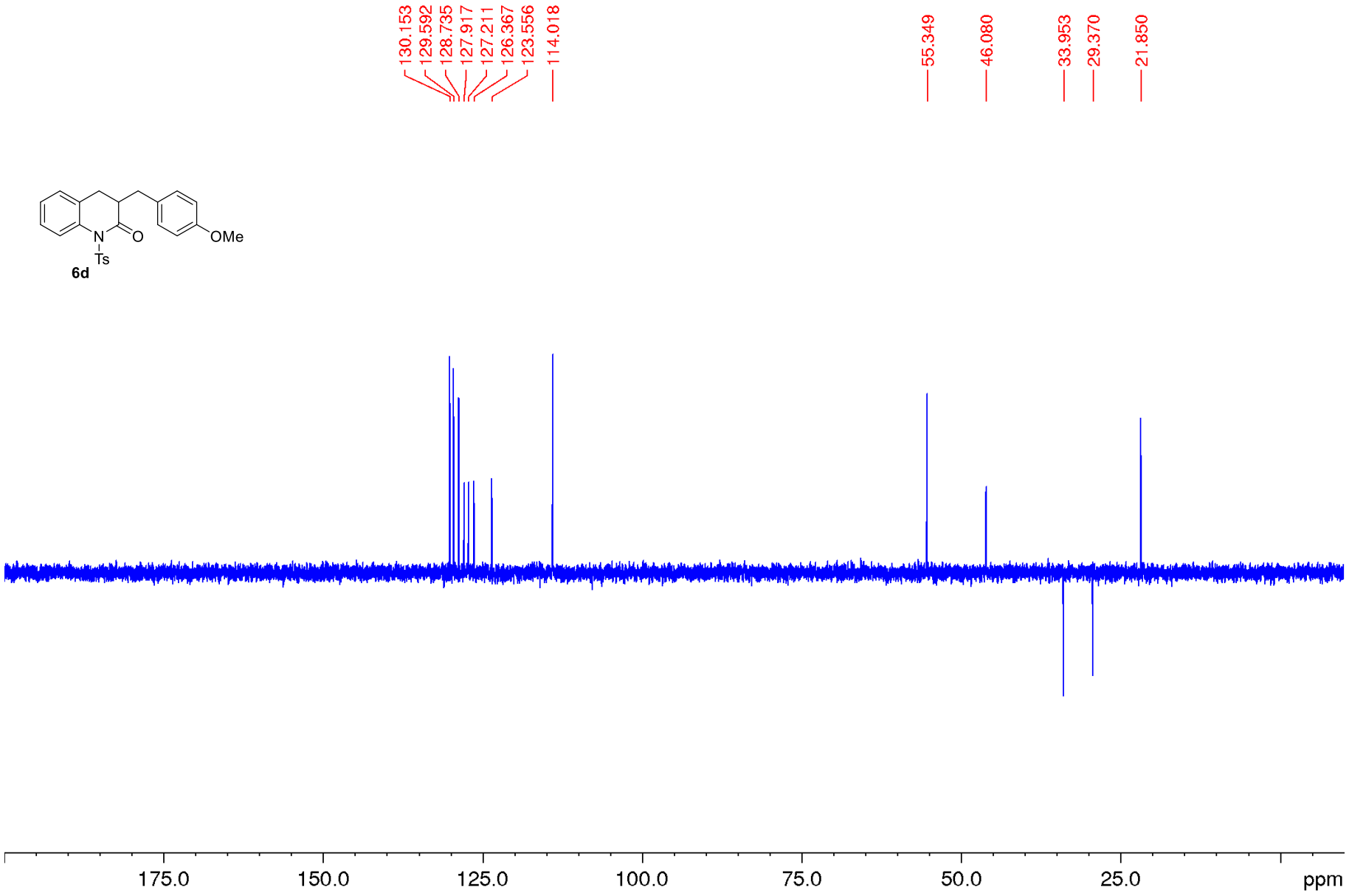
128.749
127.909
127.217
126.356
123.571
114.040
55.354
46.106
33.977
29.404
21.840
N
O
OMe
Ts
6d
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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OMe
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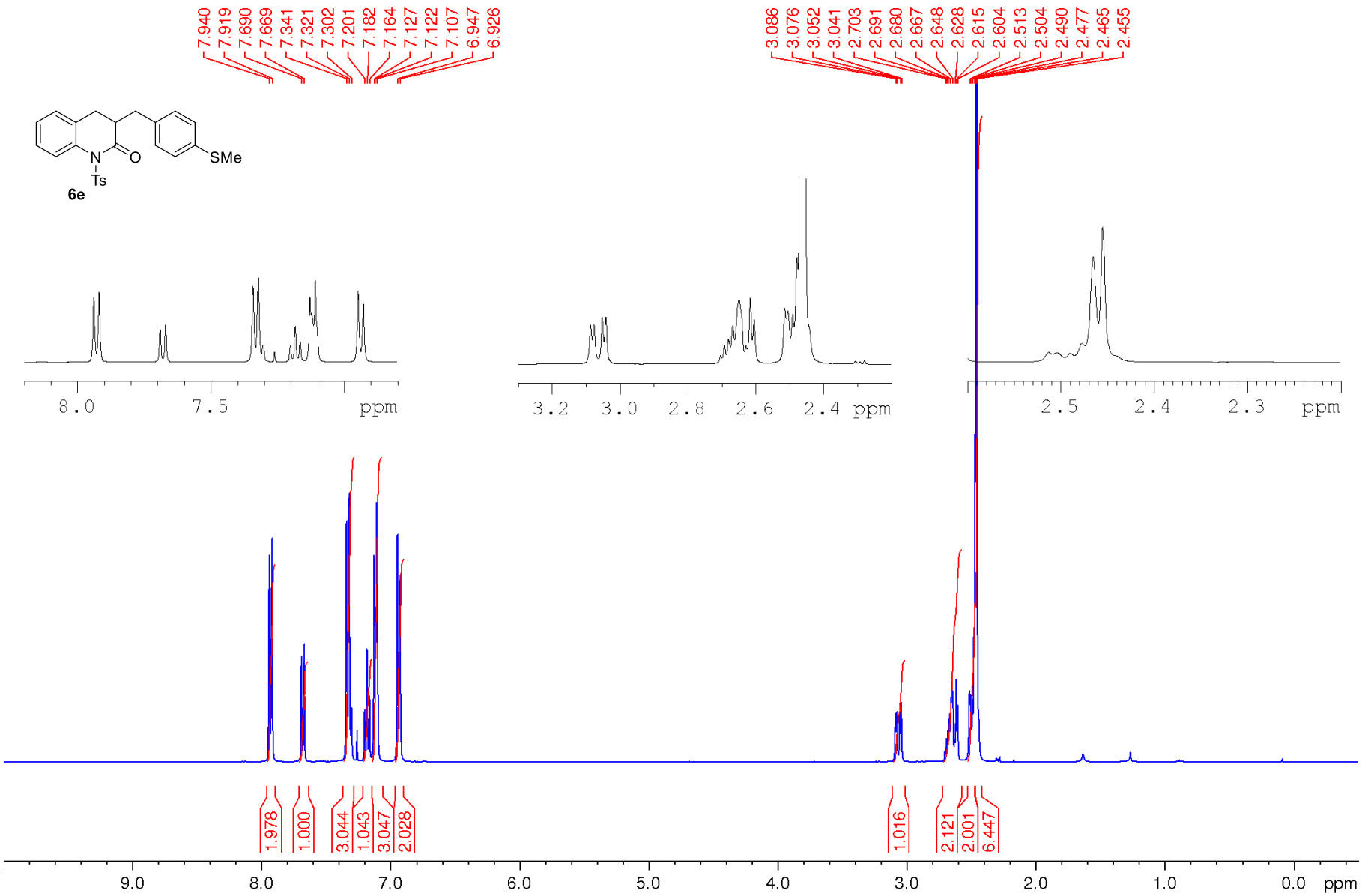
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7.107
6.947
6.926
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3.076
3.052
3.041
2.703
2.691
2.680
2.667
2.648
2.628
2.615
2.604
2.513
2.504
2.490
2.477
2.465
2.455
N
O
Ts
SMe
6e
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7.5
ppm
3.2
3.0
2.8
2.6
2.4
ppm
2.5
2.4
2.3
ppm
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1.000
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1.043
3.047
2.028
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2.121
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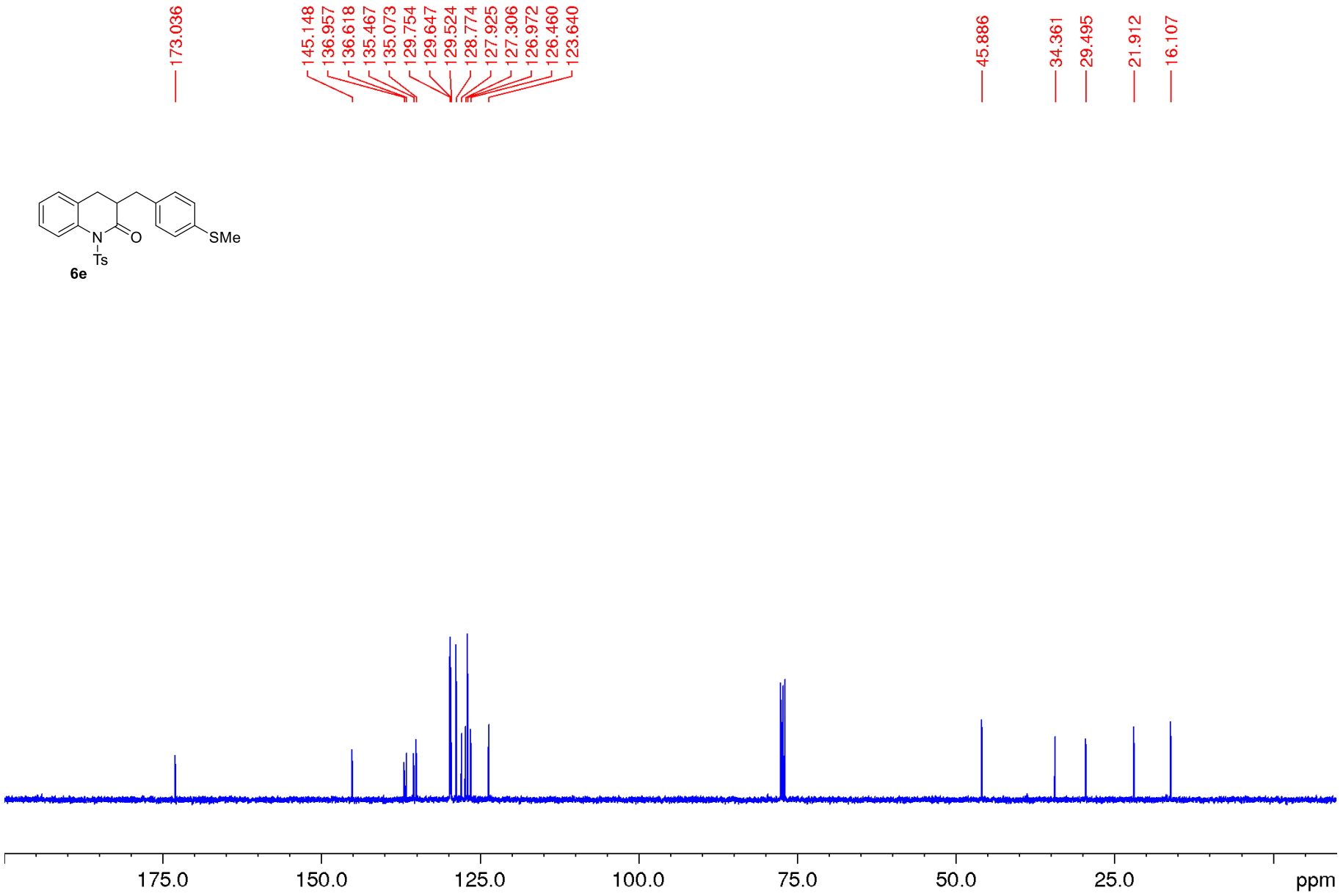
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126.460
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29.495
21.912
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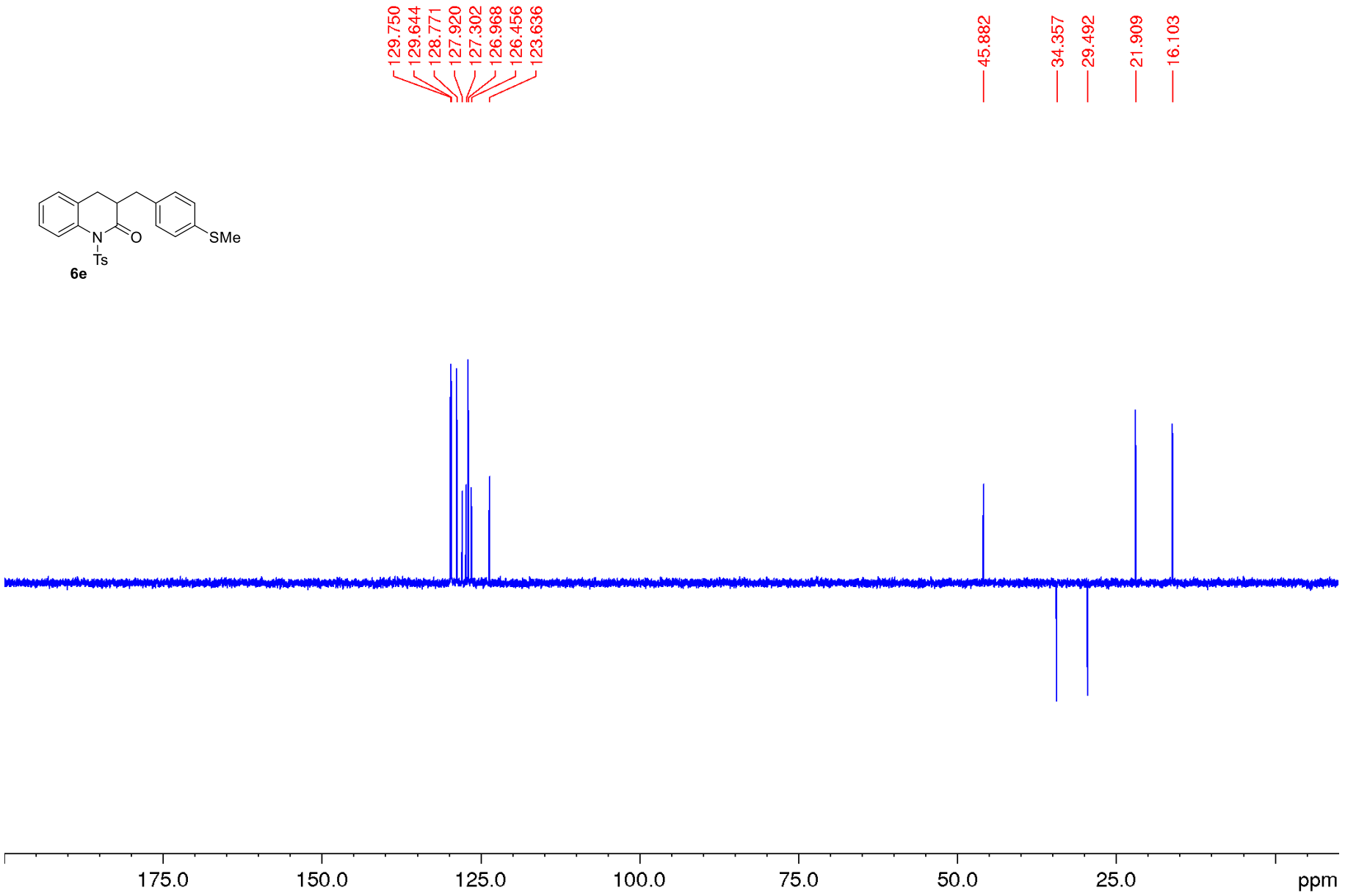
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O
Ts
SMe
6e
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25.0
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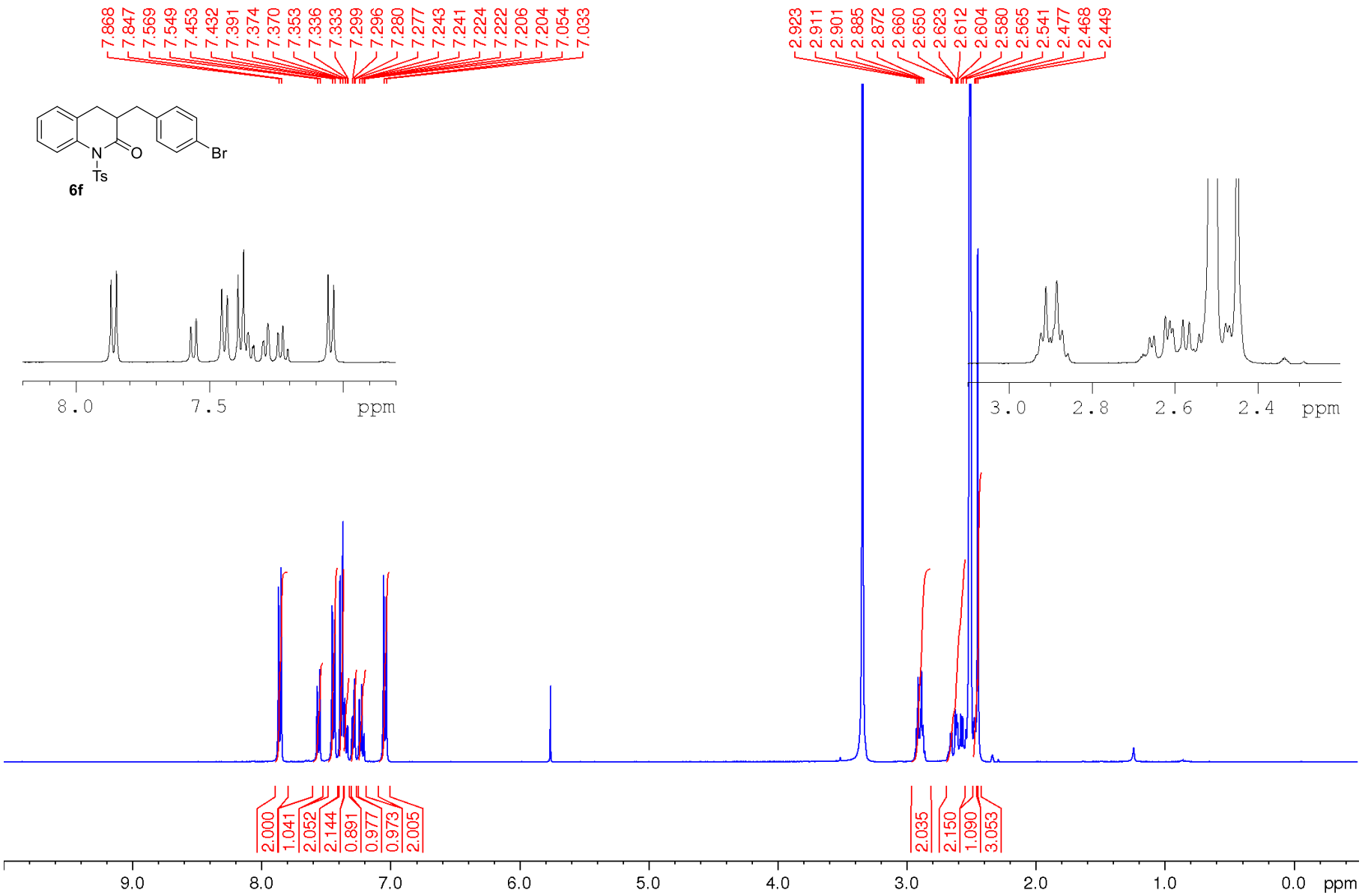
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7.299
7.296
7.280
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7.243
7.241
7.224
7.222
7.206
7.204
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7.033
2.923
2.911
2.901
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2.872
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2.623
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2.541
2.477
2.468
2.449
N
O
Br
Ts
6f
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7.5
ppm
3.0
2.8
2.6
2.4
ppm
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2.144
0.891
0.977
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2.150
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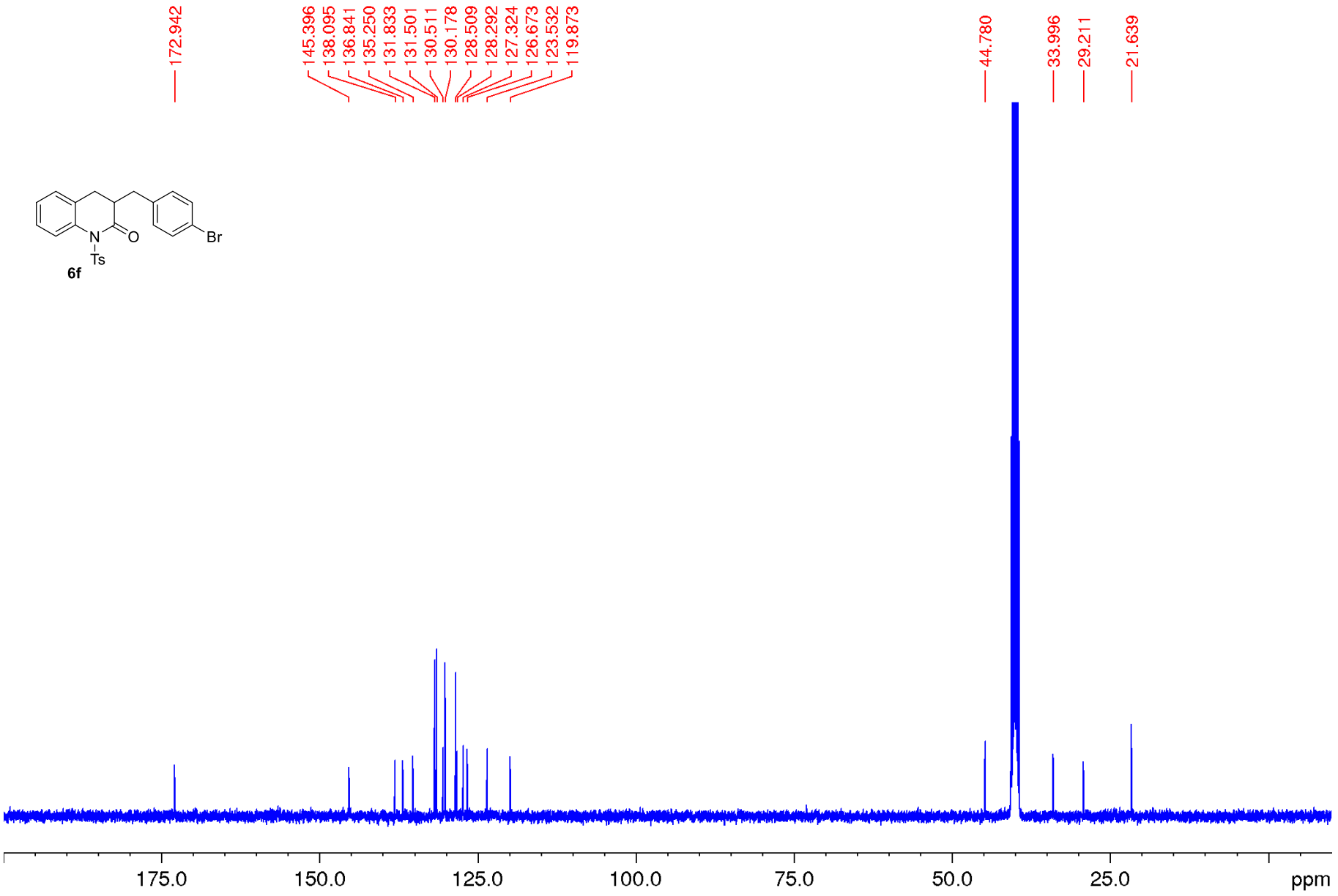
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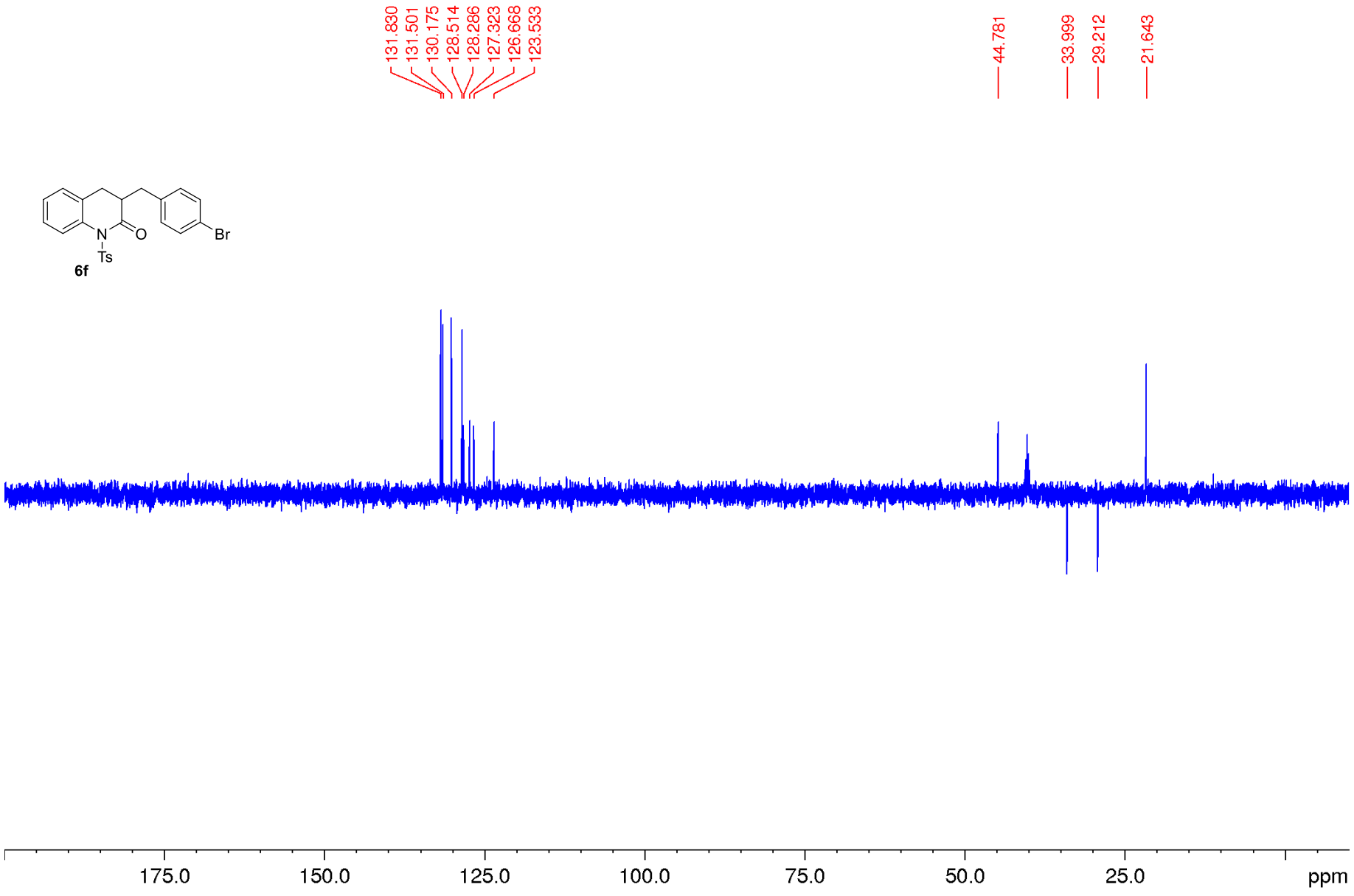
126.673
123.532
119.873
44.780
33.996
29.211
21.639
N
O
Ts
Br
6f
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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123.533
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O
Br
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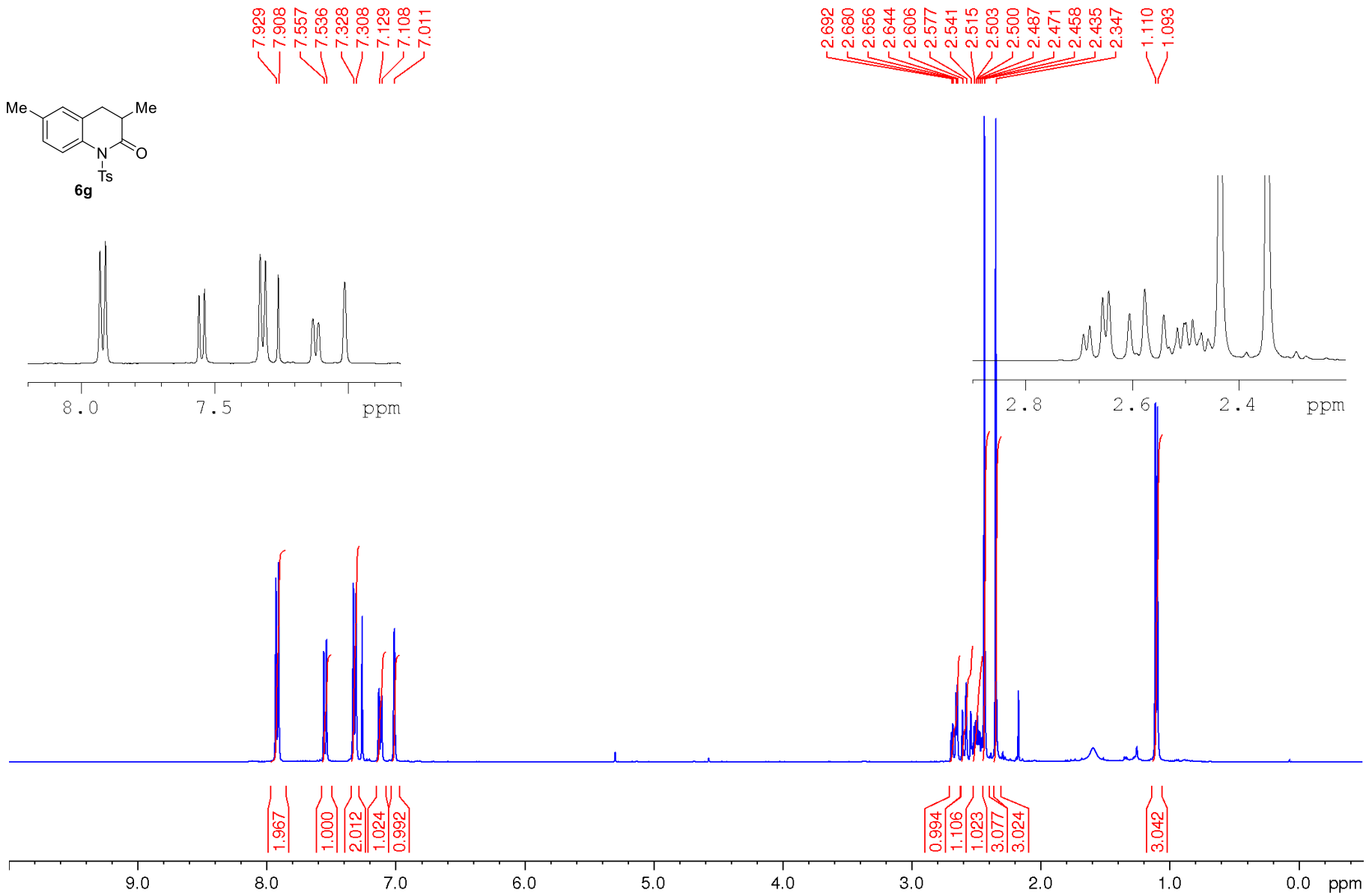
ppm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7.557
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7.328
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7.129
7.108
7.011
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2.644
2.606
2.577
2.541
2.515
2.503
2.500
2.487
2.471
2.458
2.435
2.347
1.110
1.093
Me
Me
N
O
Ts
6g
8.0
7.5
ppm
2.8
2.6
2.4
ppm
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1.000
2.012
1.024
0.992
0.994
1.106
1.023
3.077
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1.0
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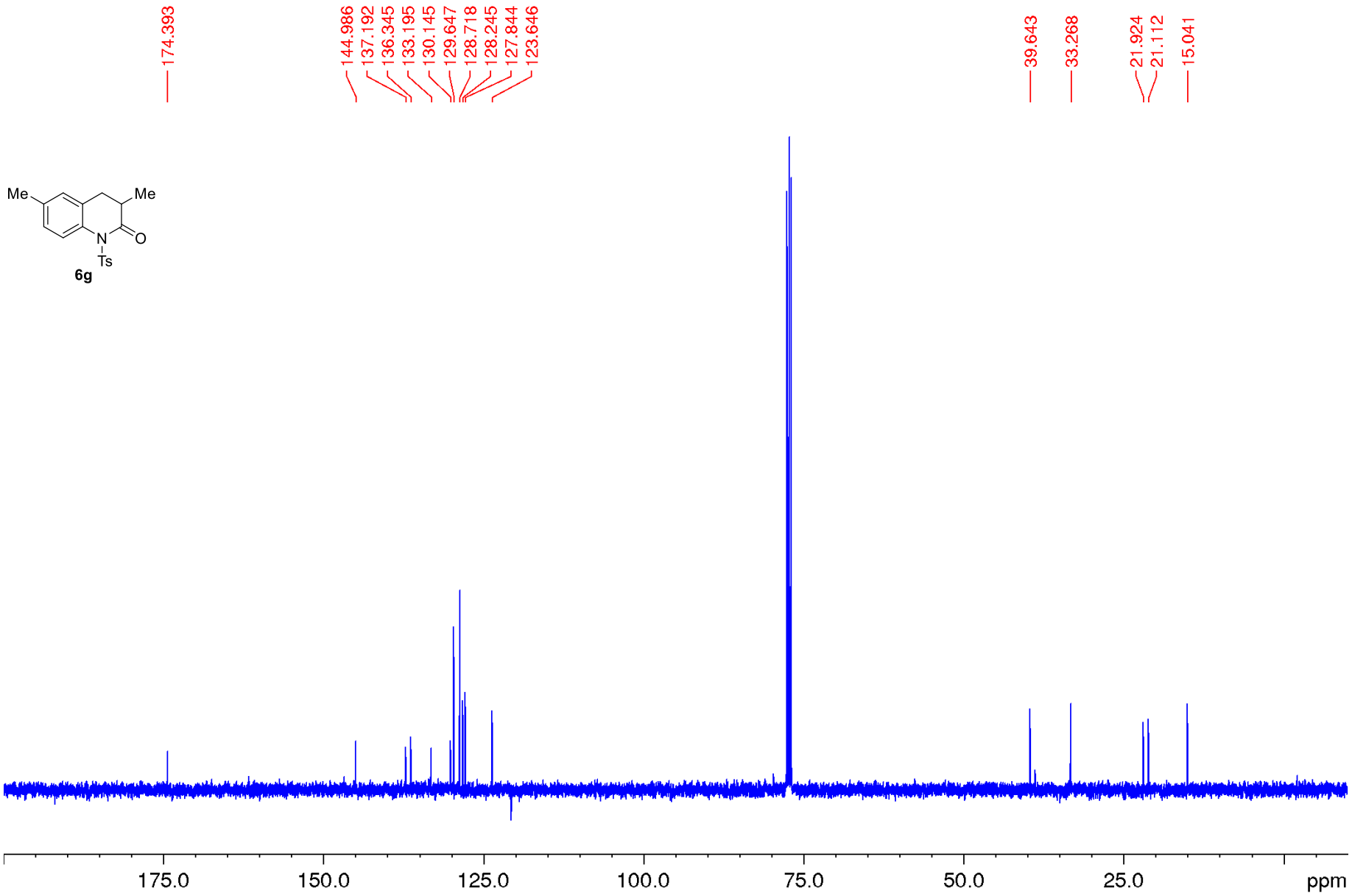
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128.718
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127.844
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39.643
33.268
21.924
21.112
15.041
Me
Me
N
O
Ts
6g
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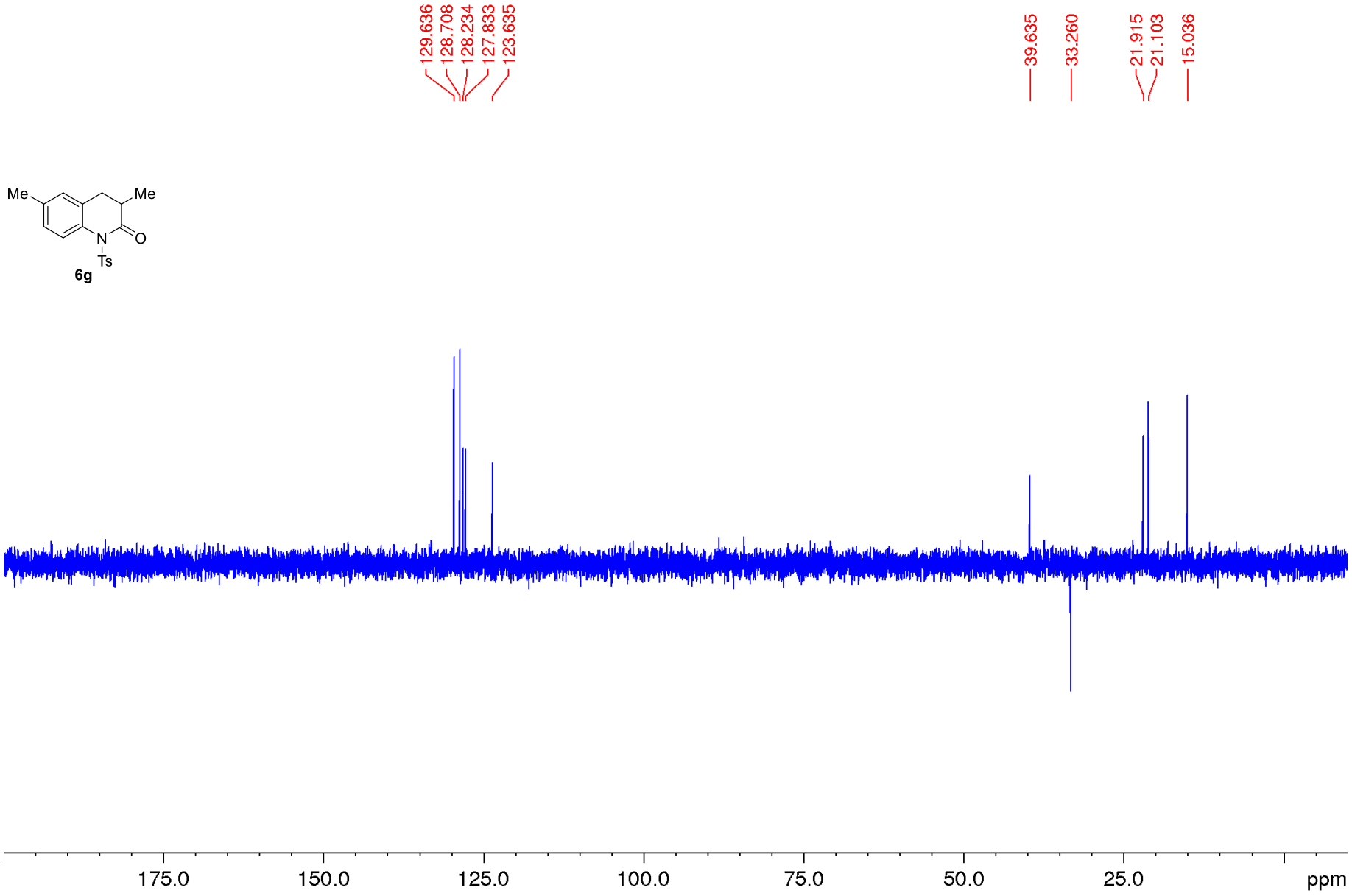
125.0
100.0
75.0
50.0
25.0
ppm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Me
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O
Ts
6g
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100.0
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25.0
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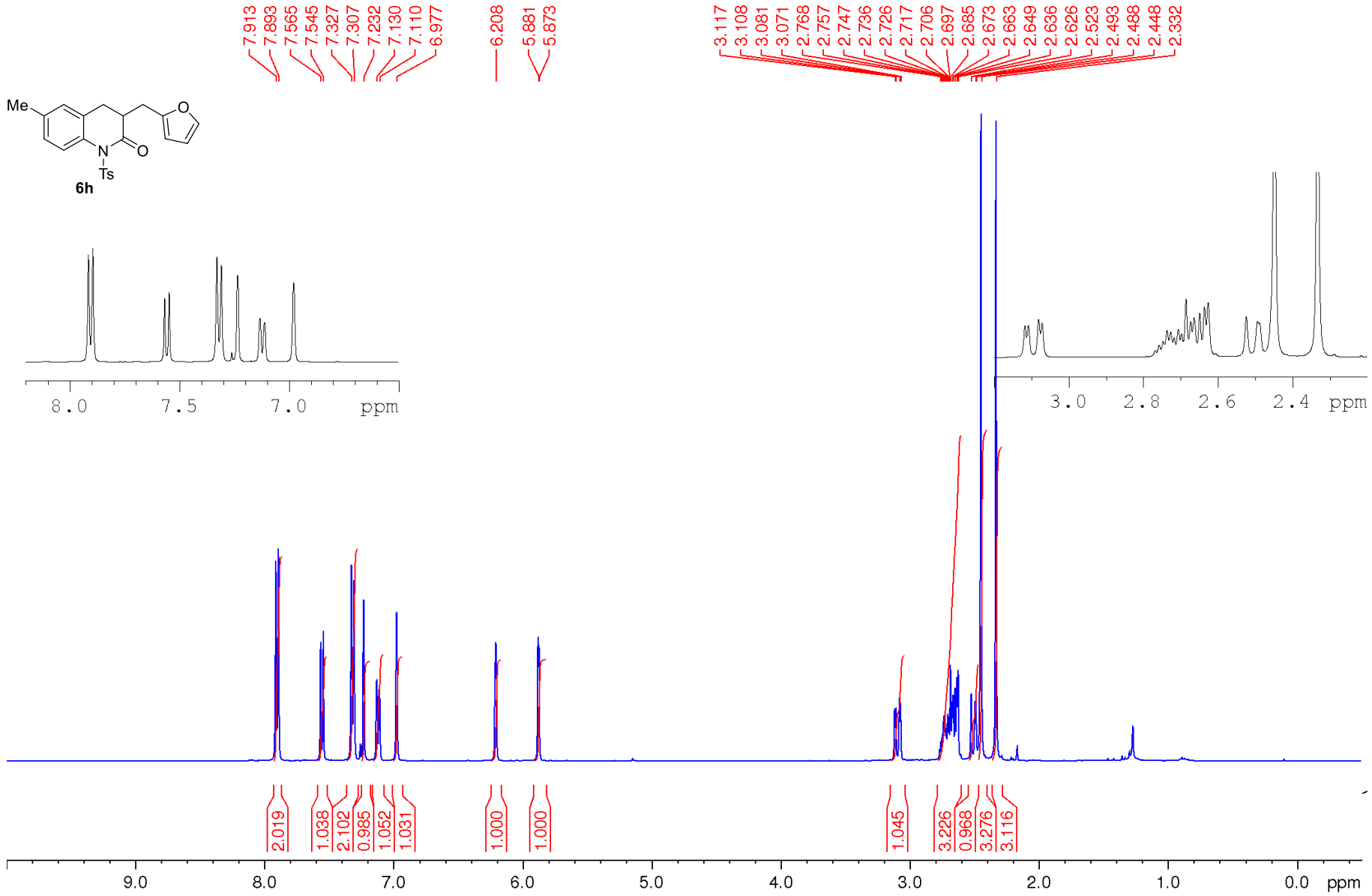
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5.873
3.117
3.108
3.081
3.071
2.768
2.757
2.747
2.736
2.726
2.717
2.706
2.697
2.685
2.673
2.663
2.649
2.636
2.626
2.523
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2.488
2.448
2.332
Me
O
N
O
Ts
6h
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7.5
7.0
ppm
3.0
2.8
2.6
2.4
ppm
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1.038
2.102
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1.052
1.031
1.000
1.000
1.045
3.226
0.968
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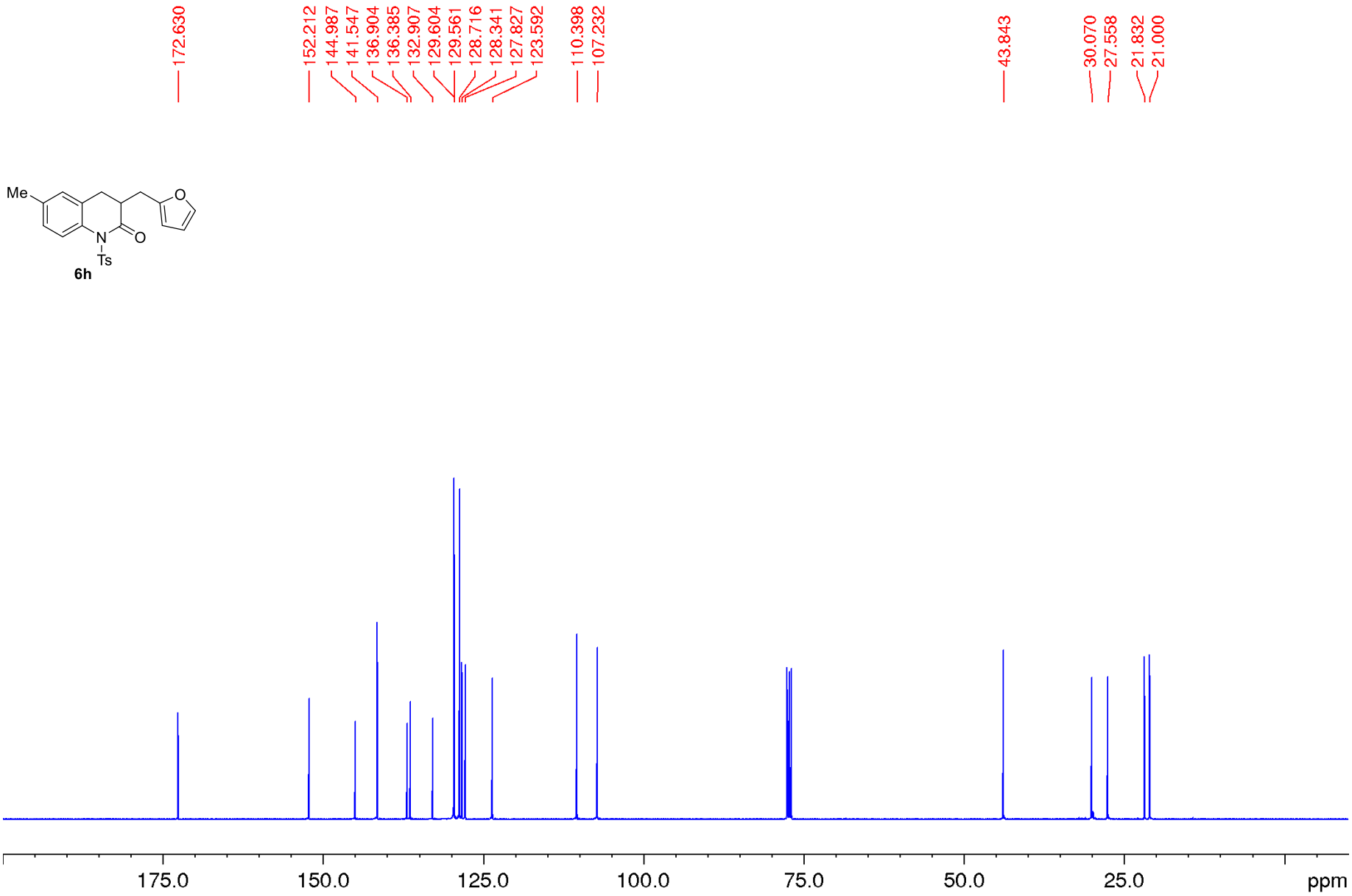
ppm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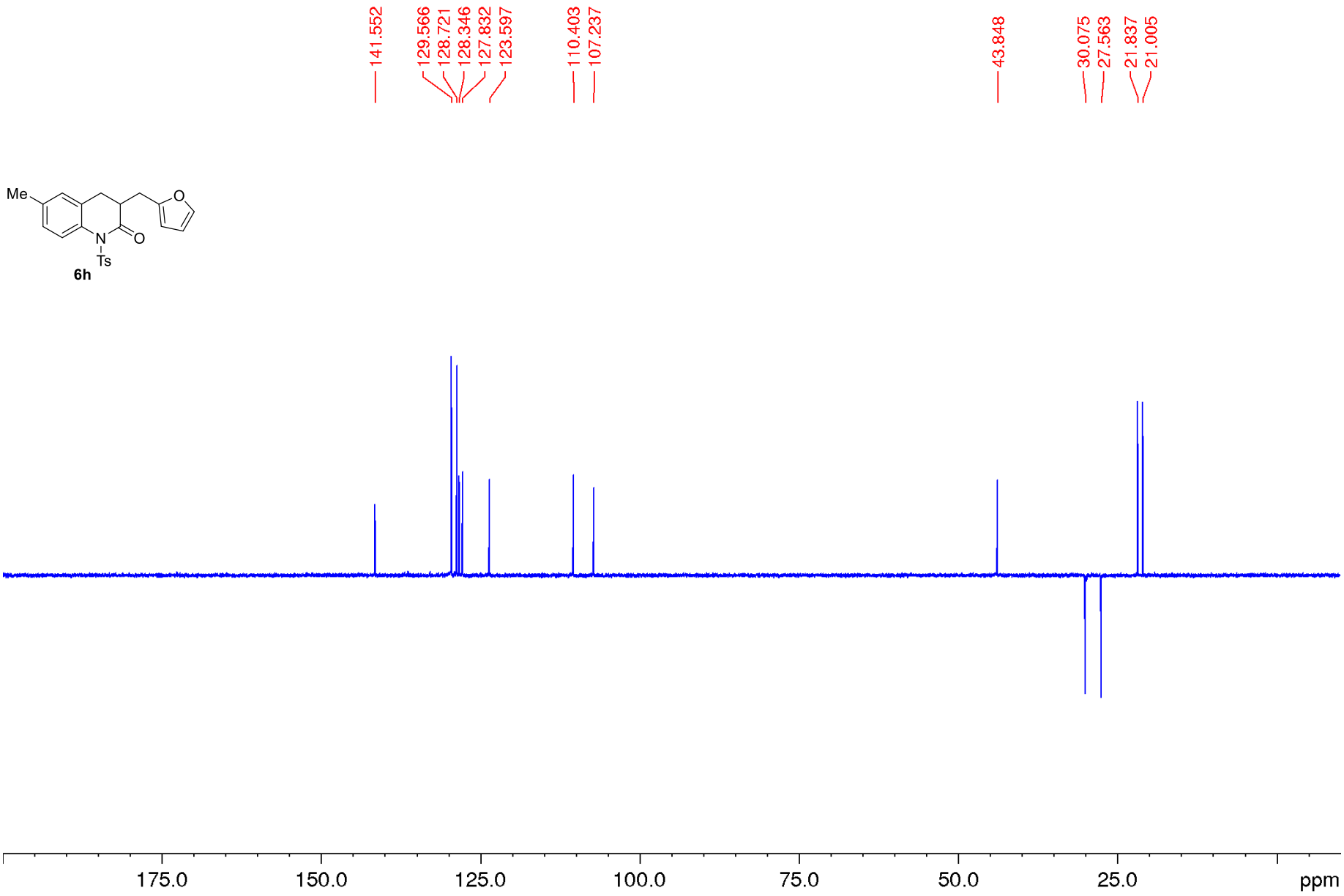
128.341
127.827
123.592
110.398
107.232
43.843
30.070
27.558
21.832
21.000
Me
O
N
O
Ts
6h
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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N
O
Ts
6h
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100.0
75.0
50.0
25.0
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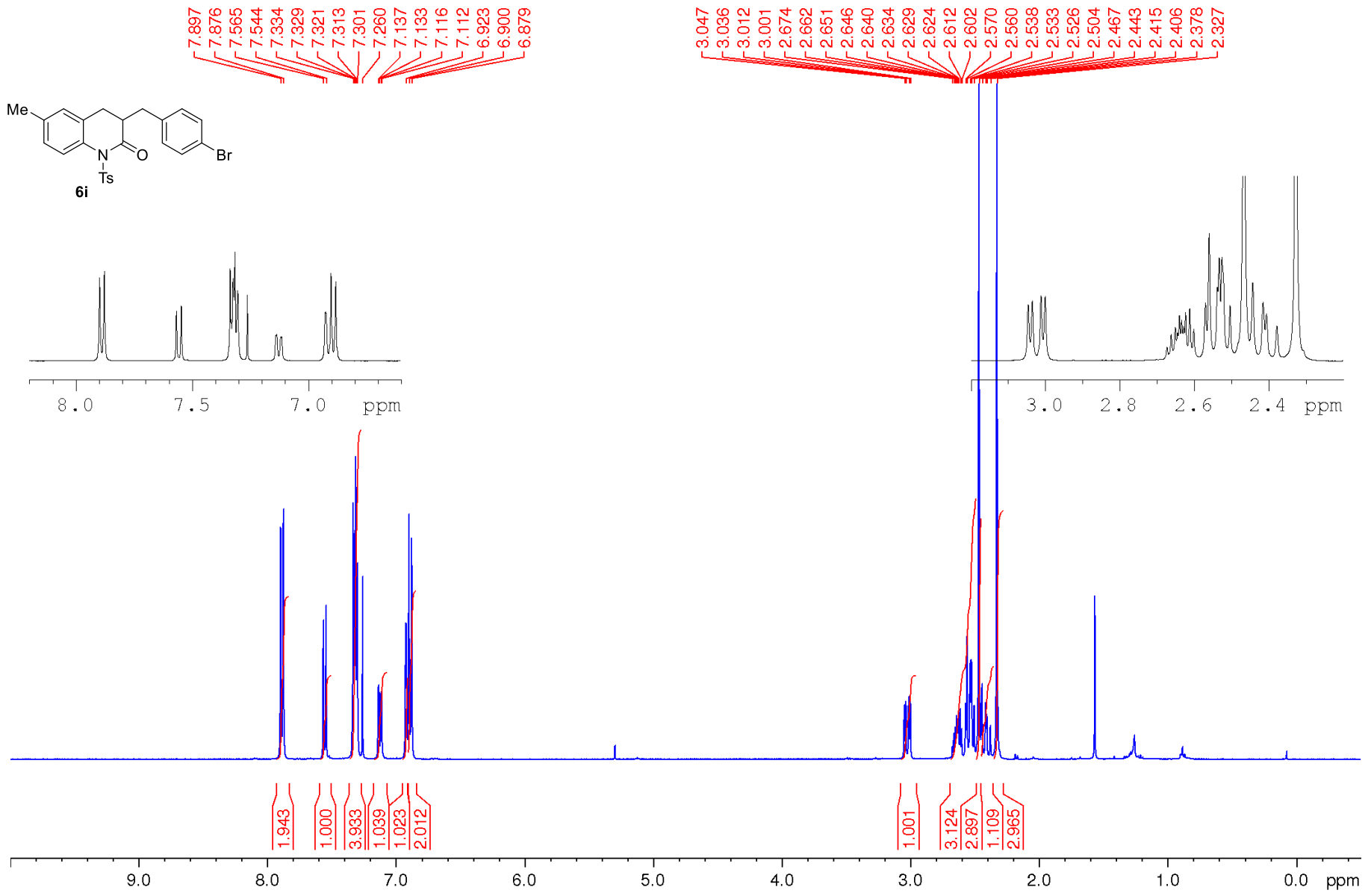
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7.112
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6.900
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2.526
2.504
2.467
2.443
2.415
2.406
2.378
2.327
Me
N
O
Br
Ts
6i
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7.0
ppm
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2.8
2.6
2.4
ppm
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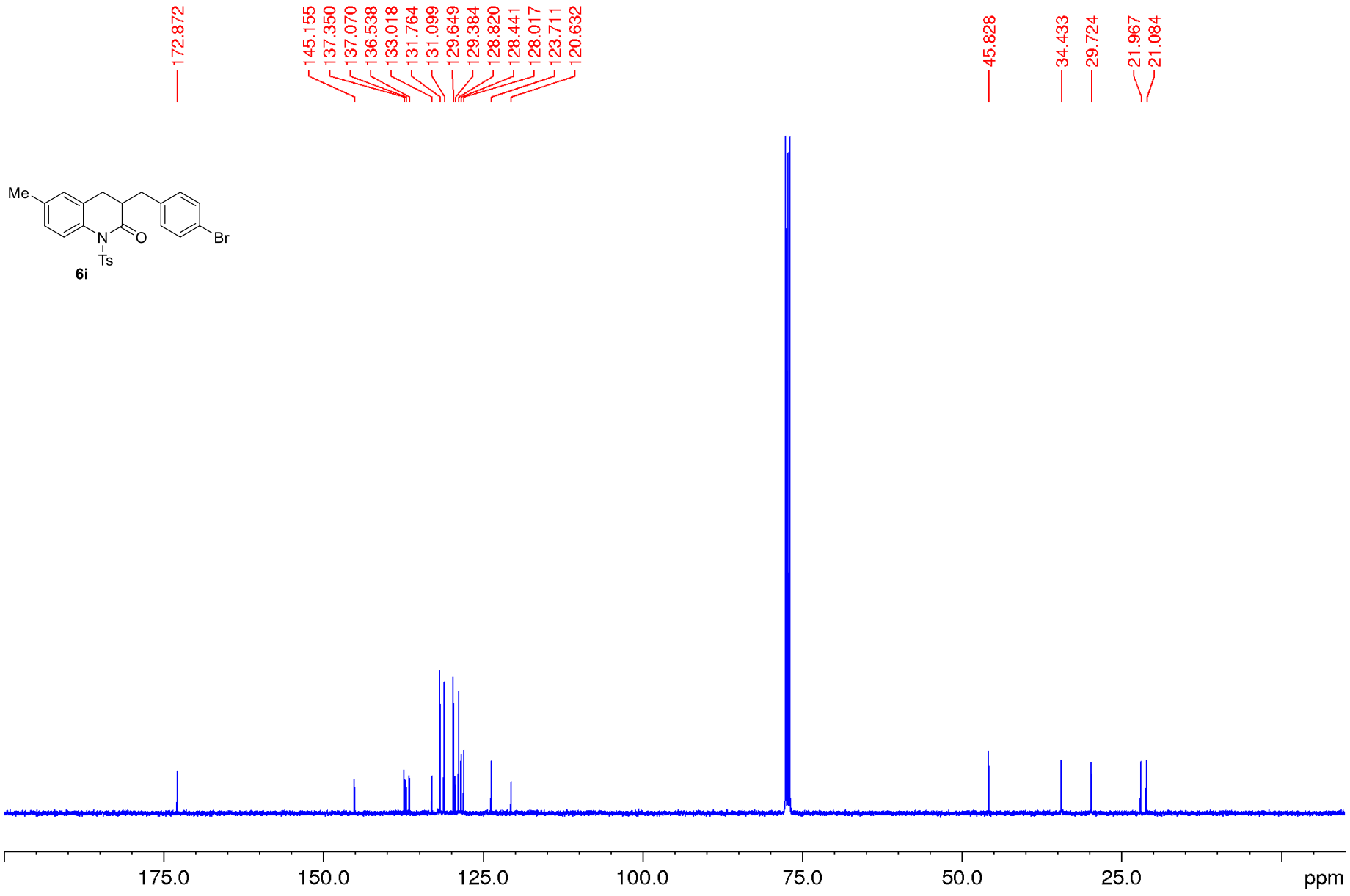
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123.711
120.632
45.828
34.433
29.724
21.967
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Me
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O
Br
Ts
6i
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150.0
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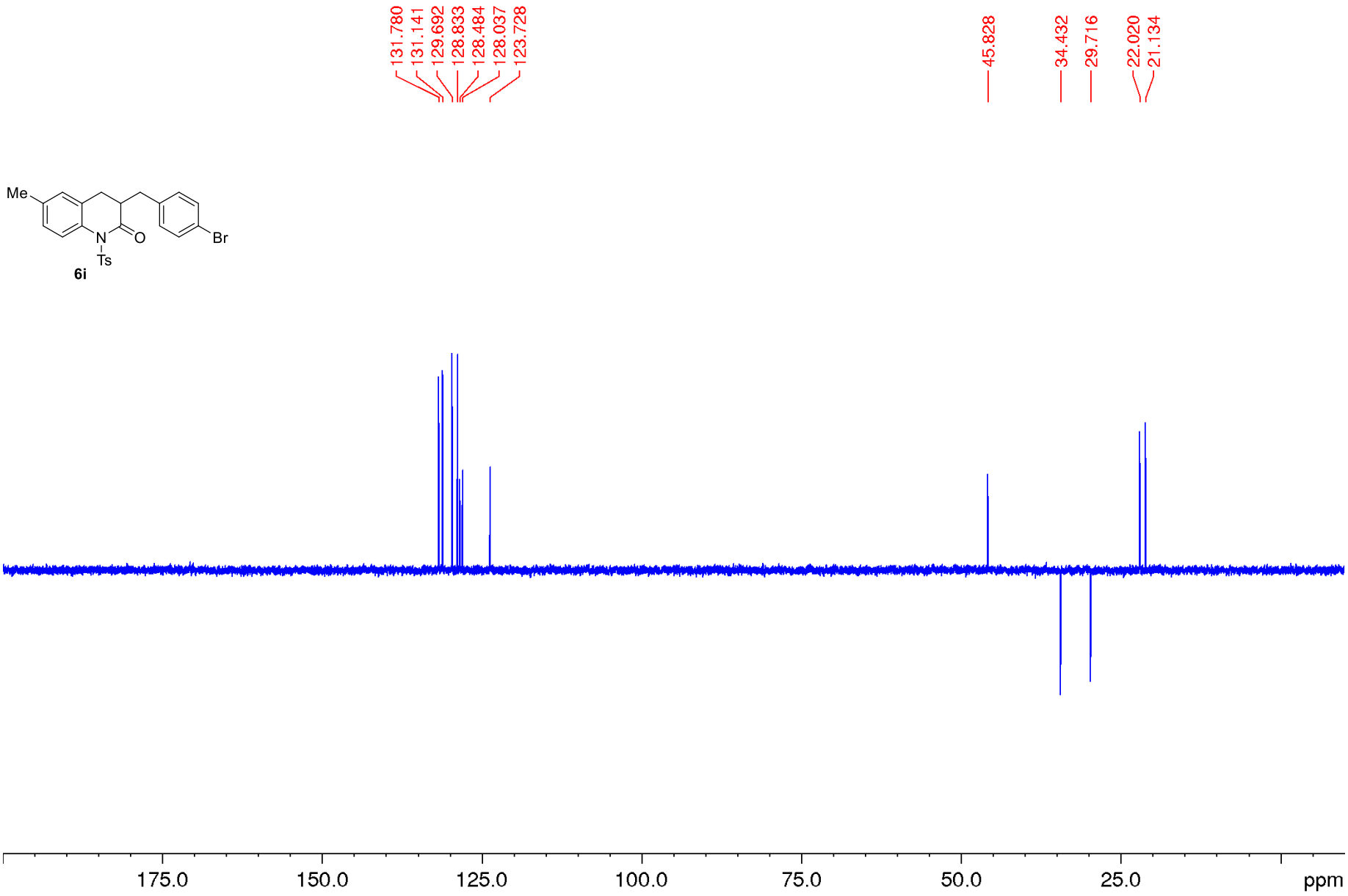
50.0
25.0
ppm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Br
Ts
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100.0
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50.0
25.0
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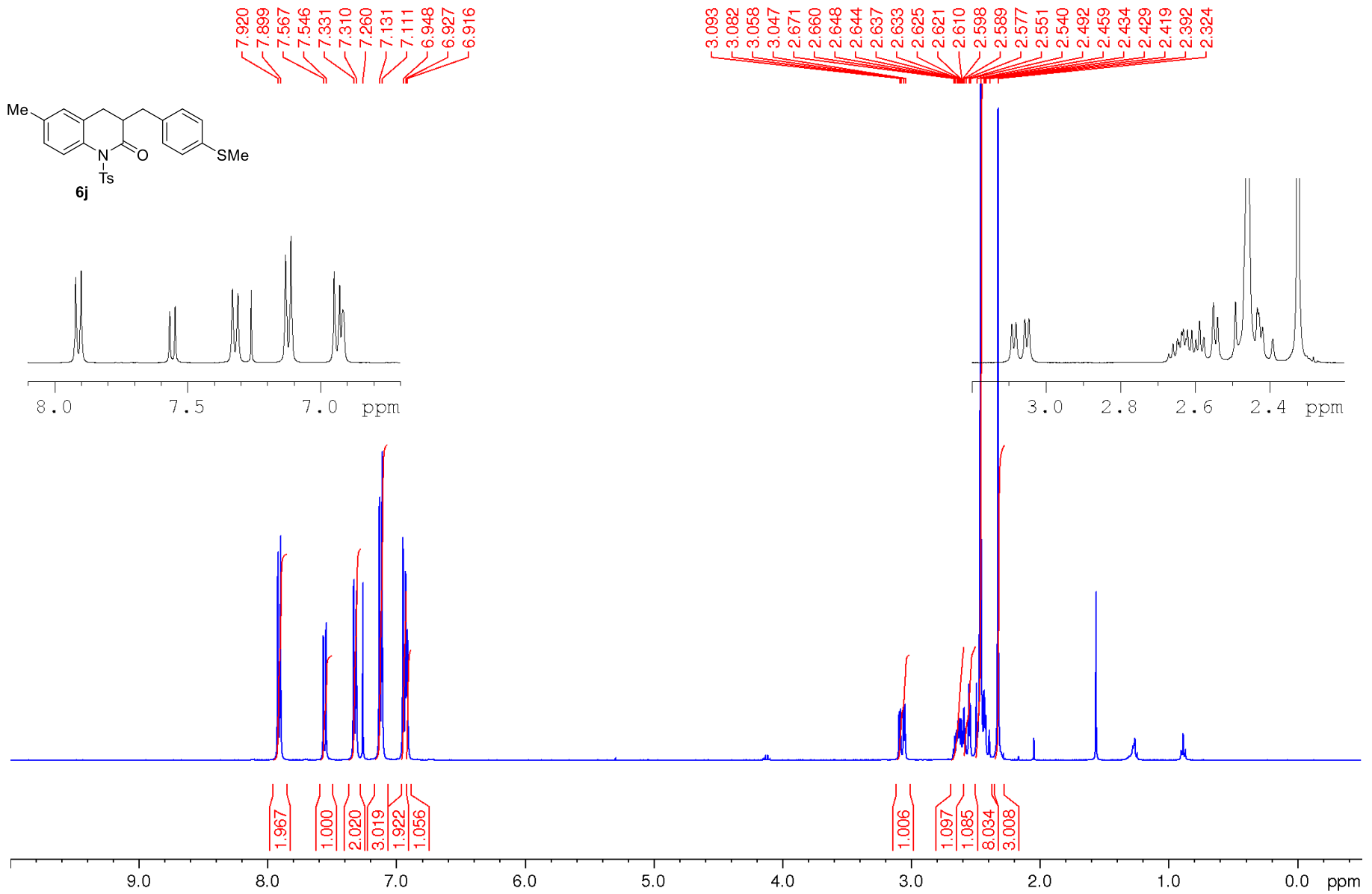
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2.429
2.419
2.392
2.324
Me
N
O
SMe
Ts
6j
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7.5
7.0
ppm
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2.8
2.6
2.4
ppm
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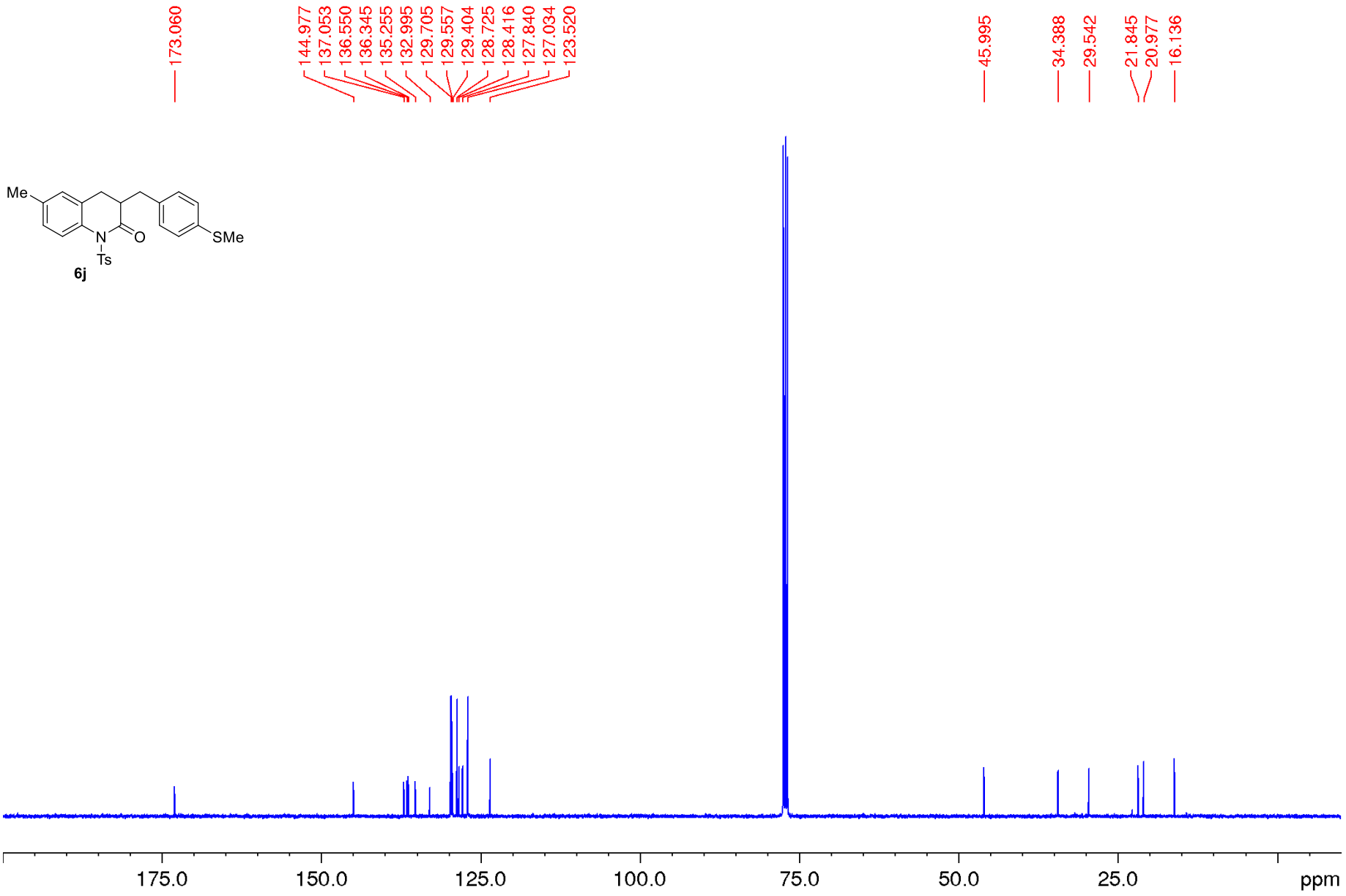
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45.995
34.388
29.542
21.845
20.977
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Ts
SMe
6j
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50.0
25.0
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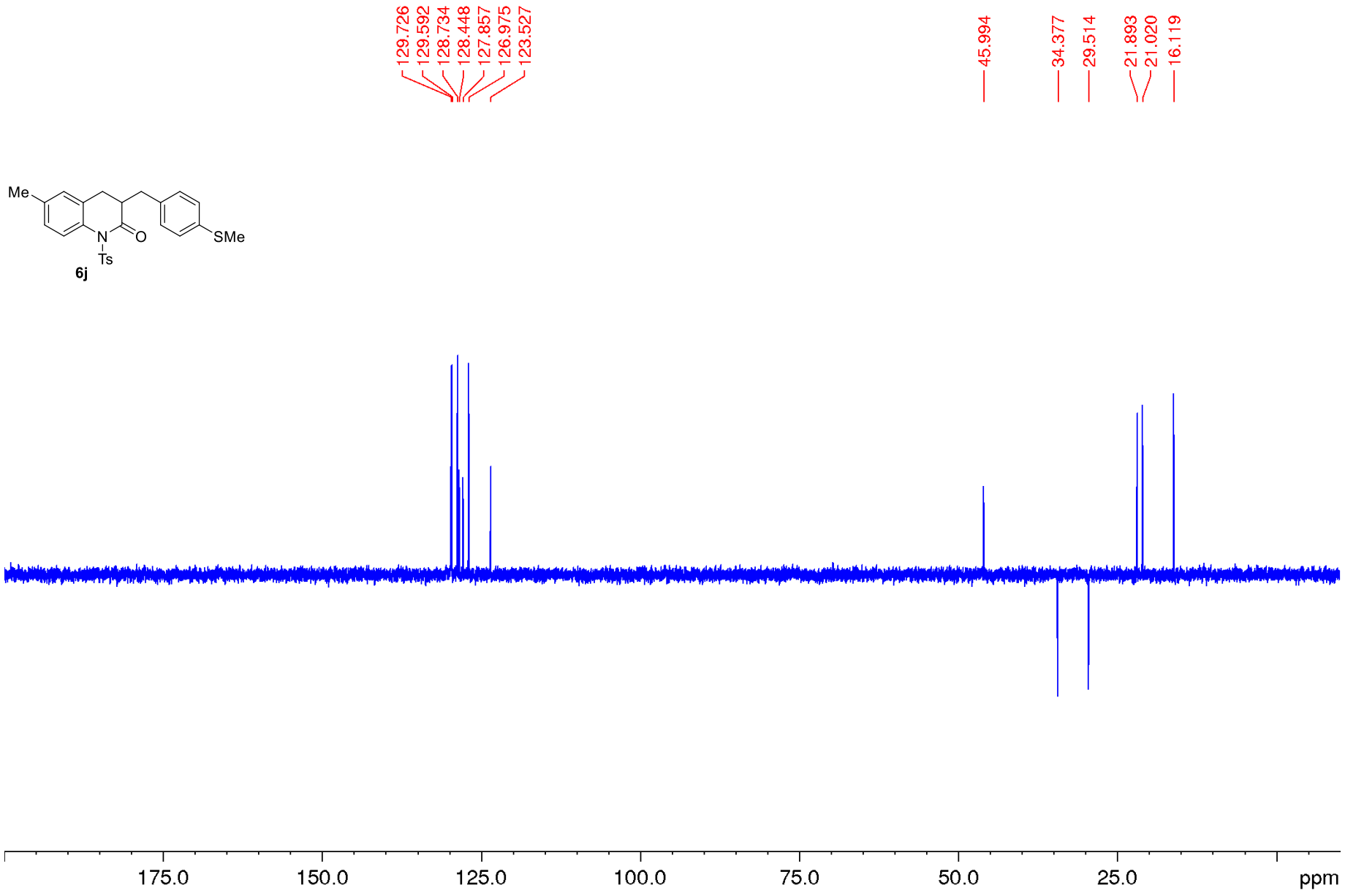
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21.020
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Ts
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6j
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50.0
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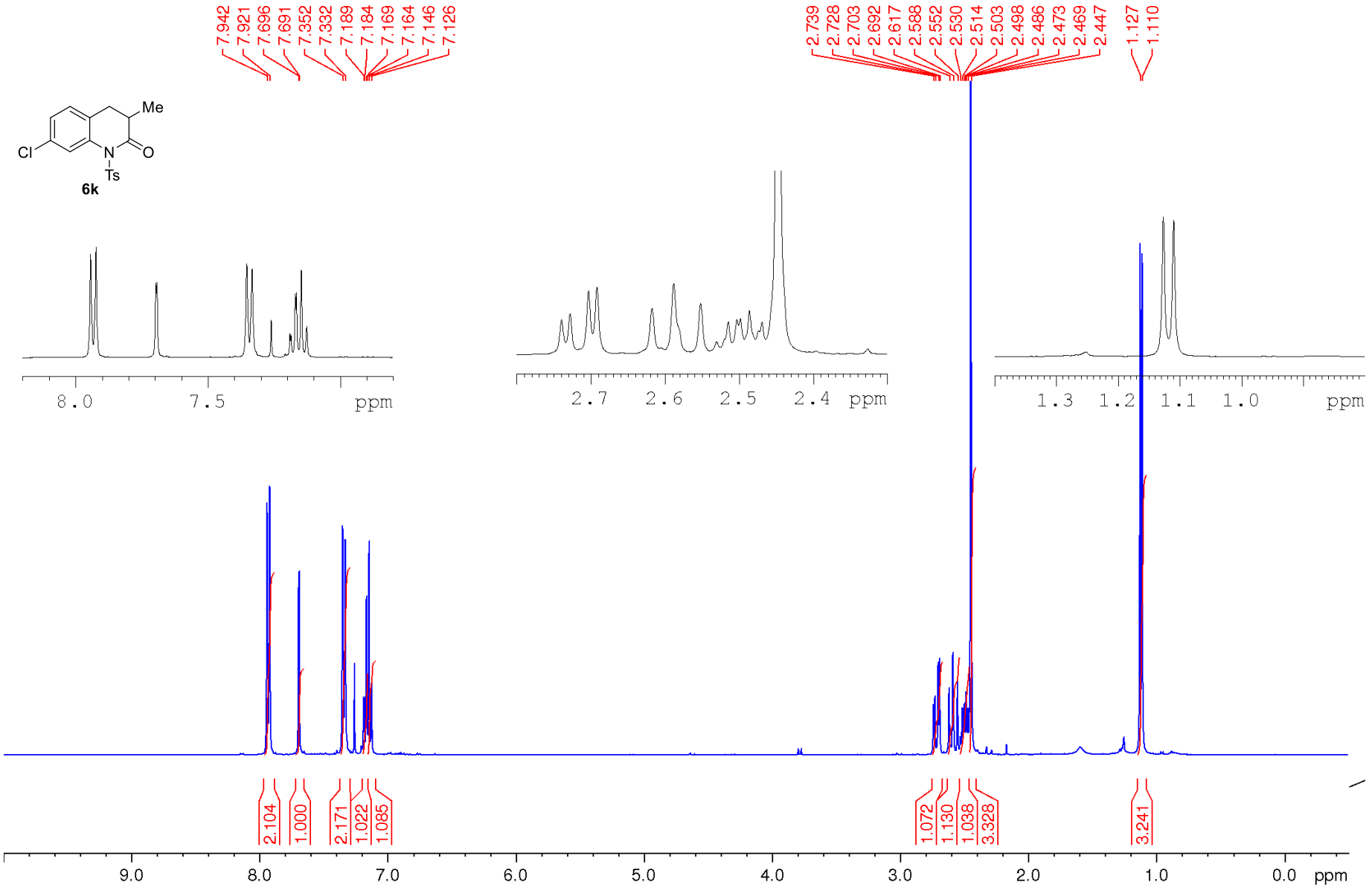
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2.703
2.692
2.617
2.588
2.552
2.530
2.514
2.503
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1.110
Me
Cl
N
O
Ts
6k
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7.5
ppm
2.7
2.6
2.5
2.4
ppm
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1.2
1.1
1.0
ppm
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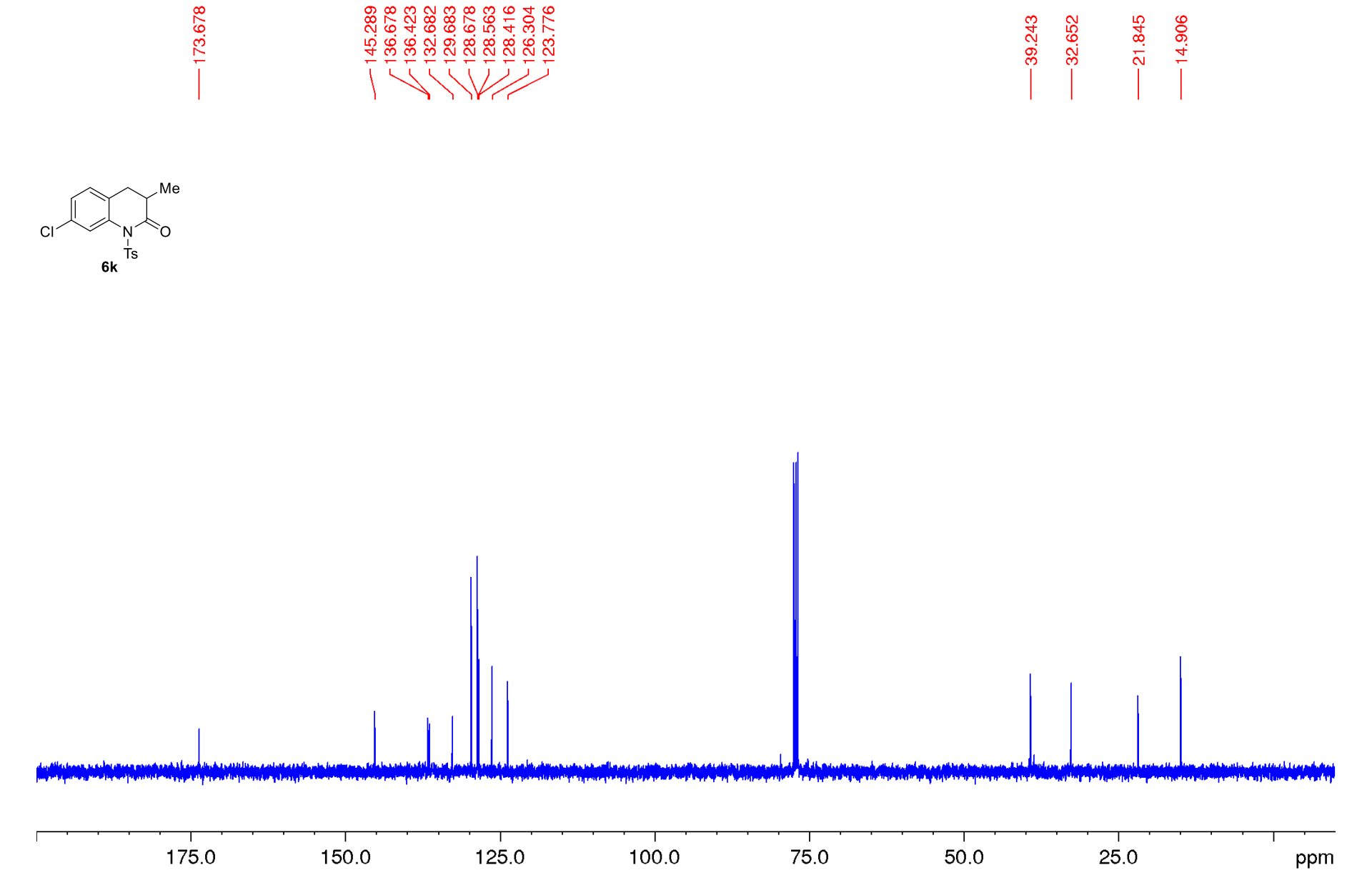
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21.845
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Ts
6k
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100.0
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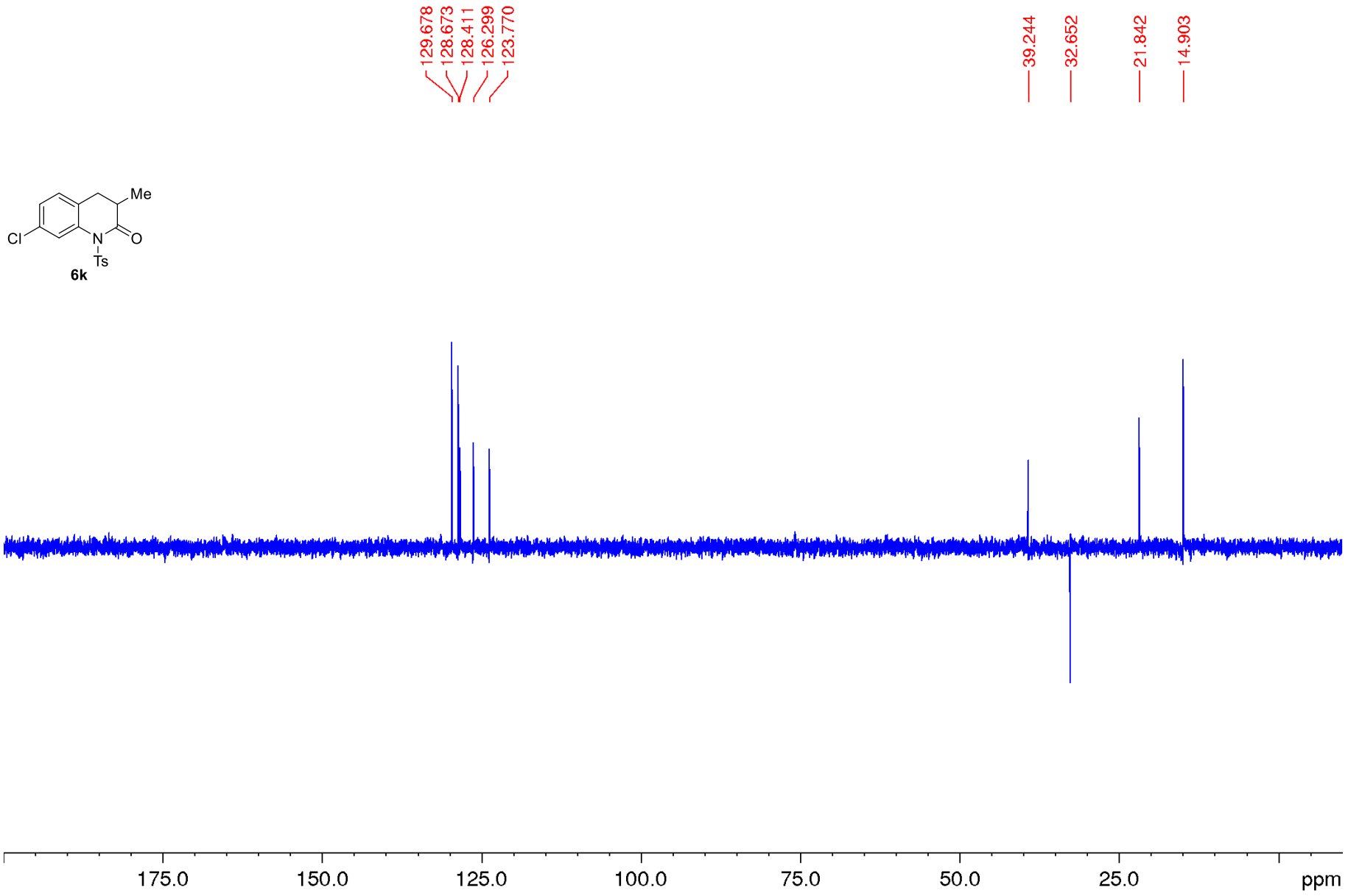
50.0
25.0
ppm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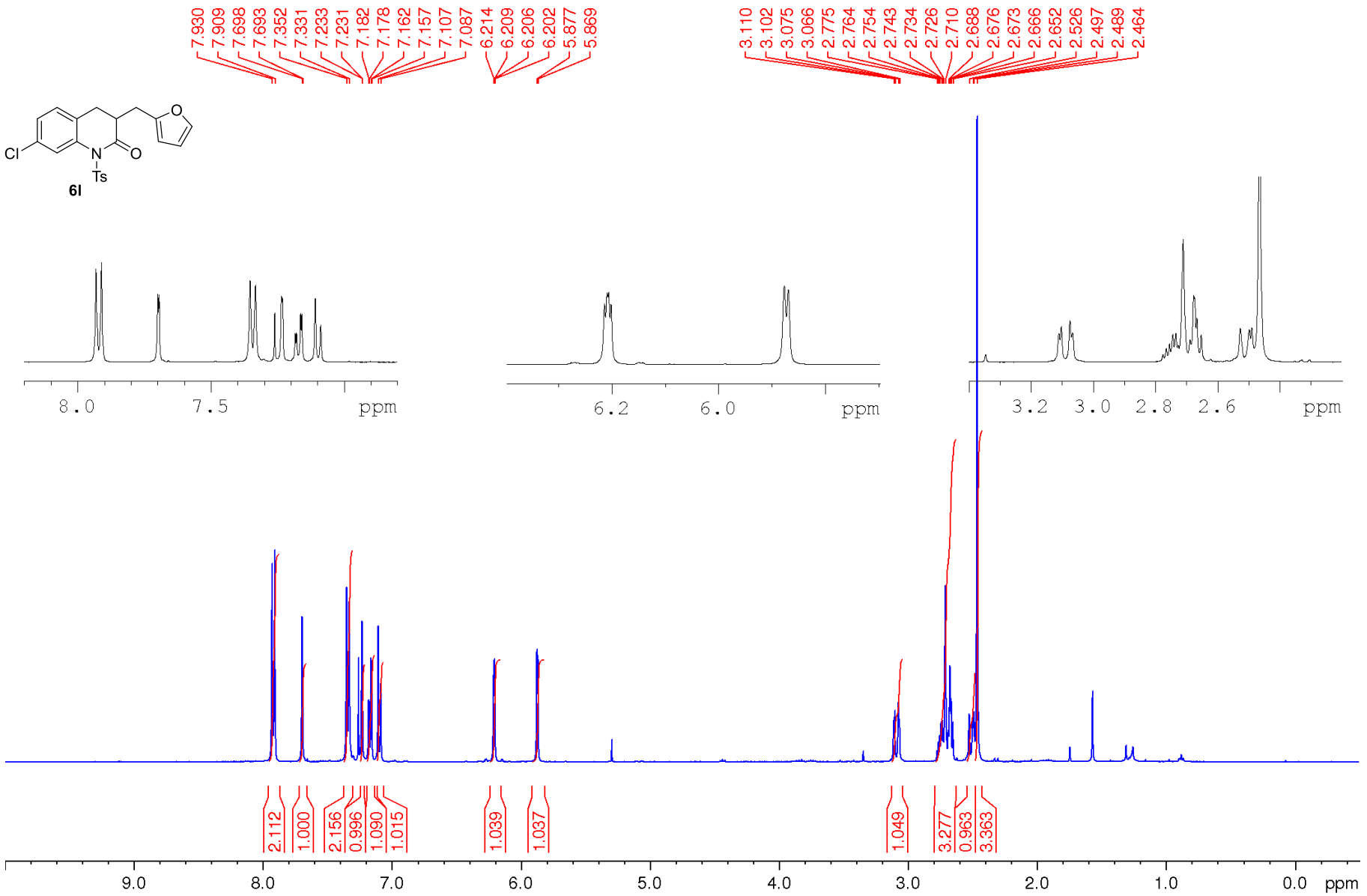
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2.734
2.726
2.710
2.688
2.676
2.673
2.666
2.652
2.526
2.497
2.489
2.464
Cl
N
O
O
Ts
6l
8.0
7.5
ppm
6.2
6.0
ppm
3.2
3.0
2.8
2.6
ppm
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1.000
2.156
0.996
1.090
1.015
1.039
1.037
1.049
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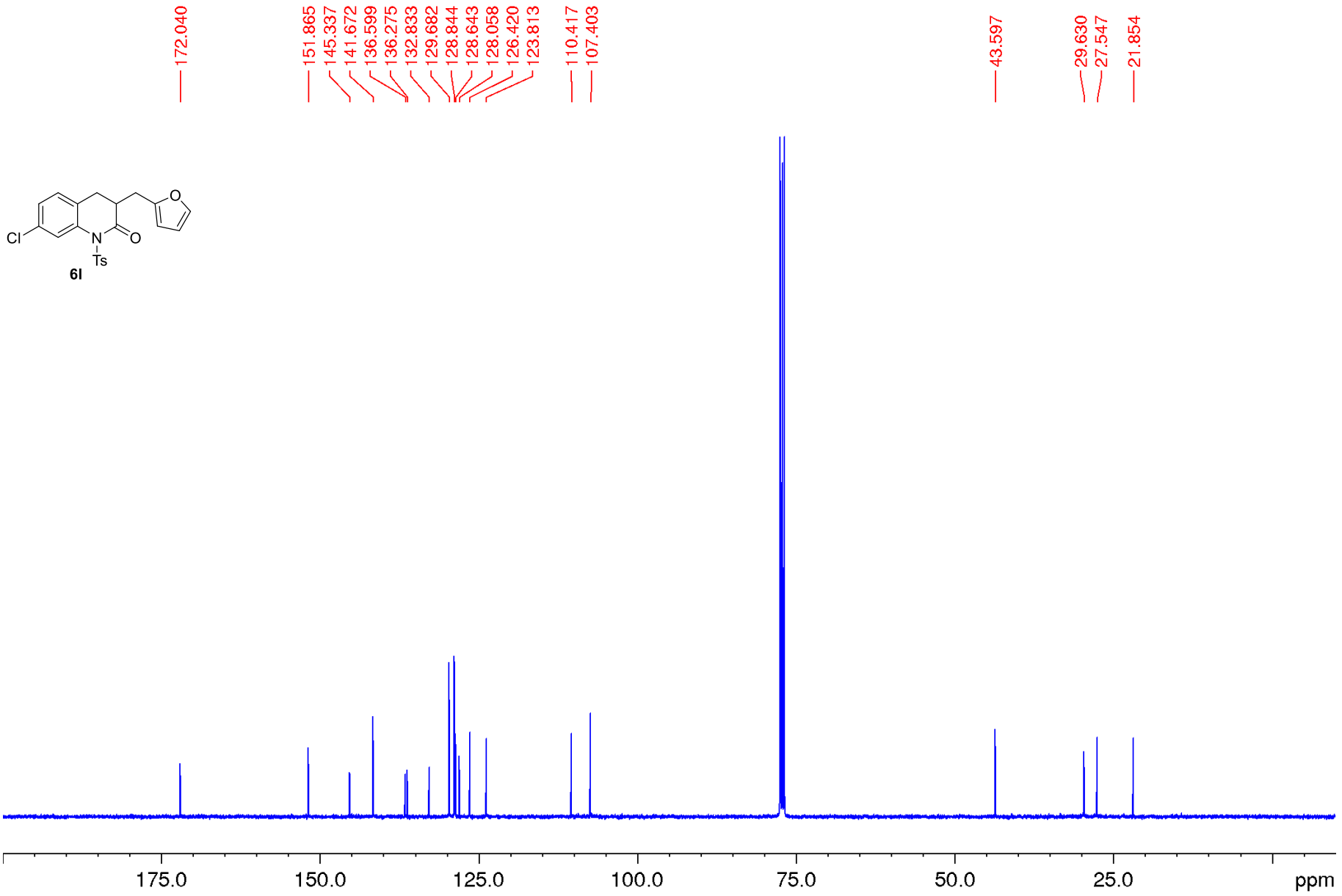
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123.813
110.417
107.403
43.597
29.630
27.547
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O
O
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25.0
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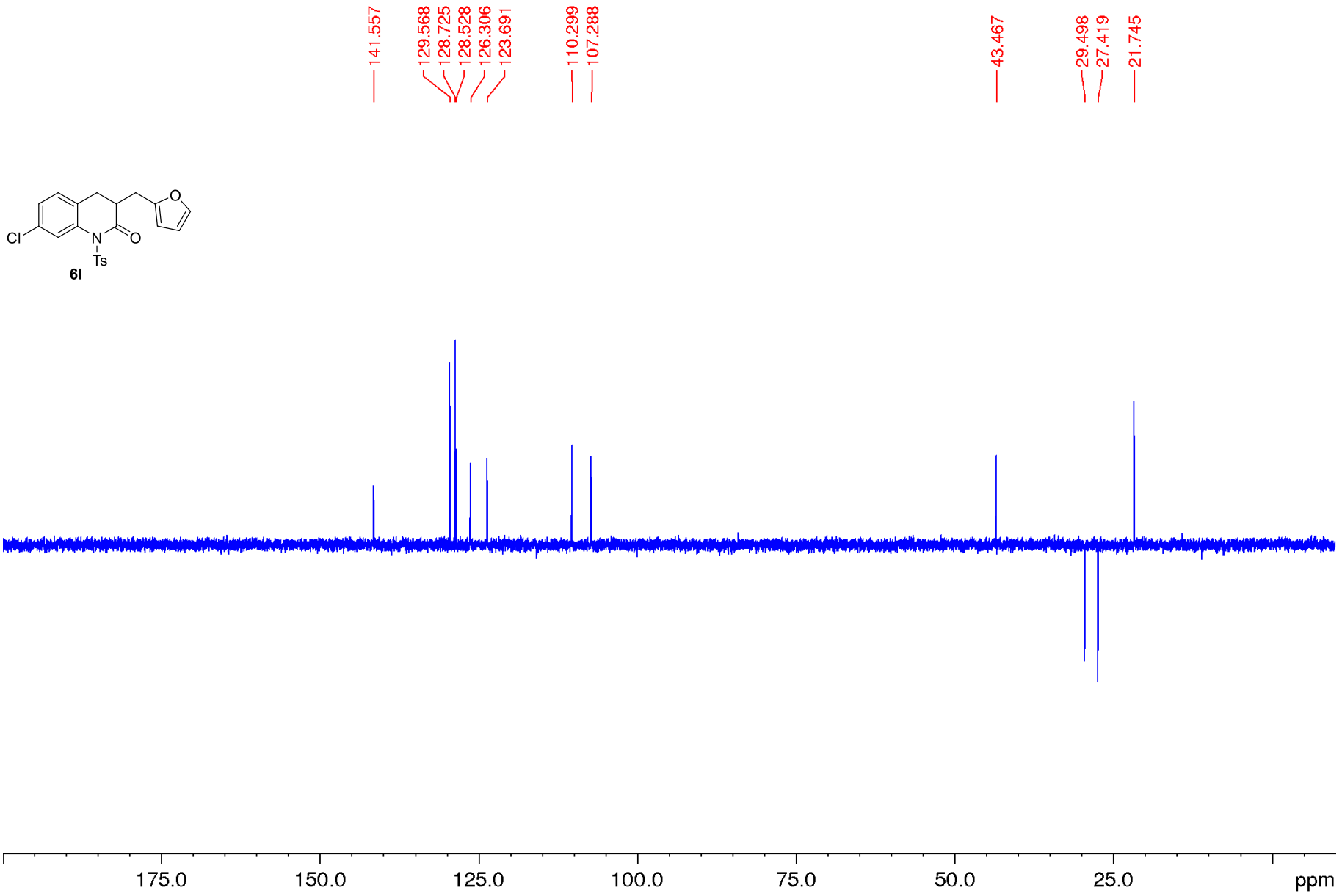
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Ts
O
O
6l
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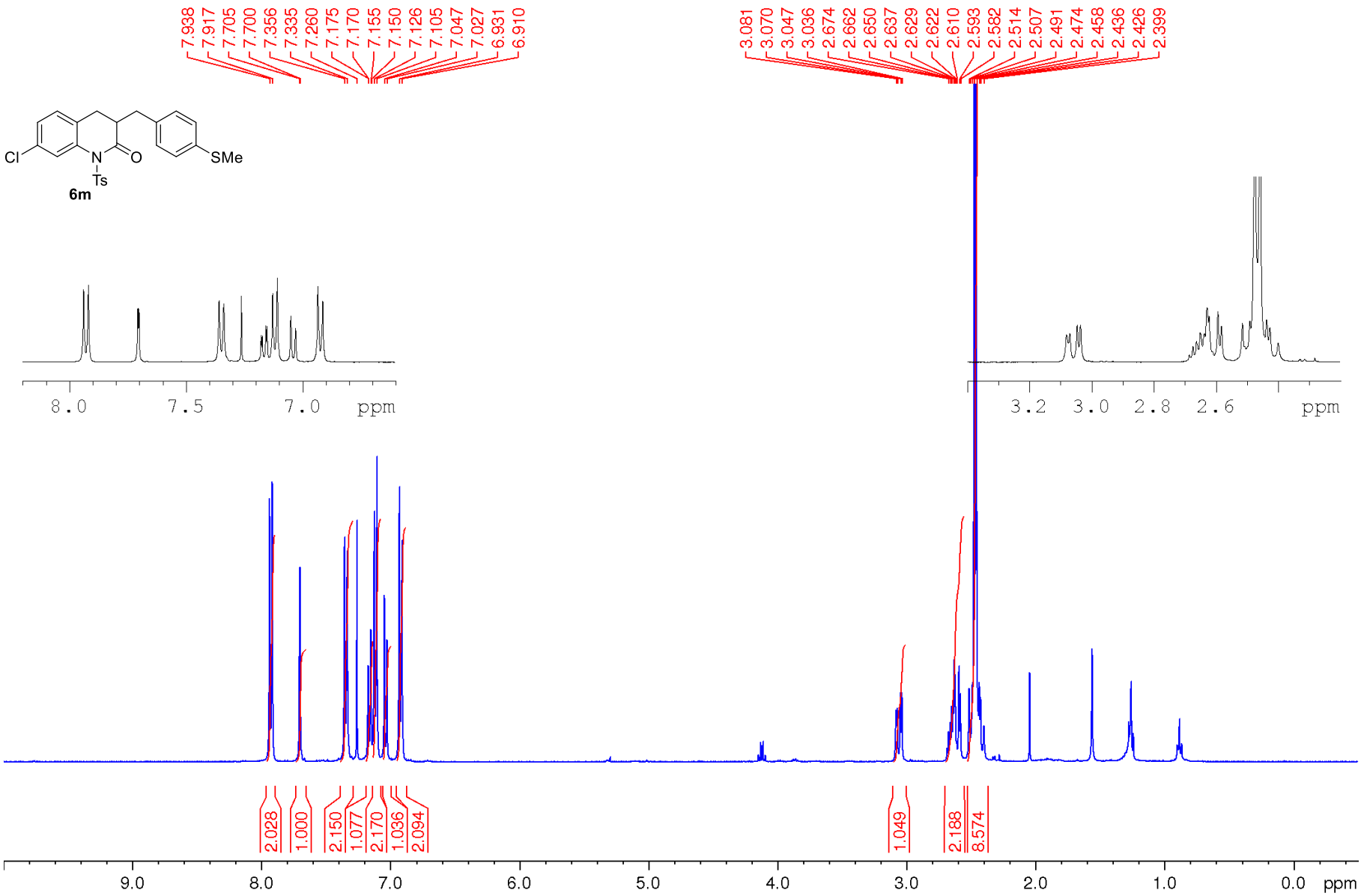
50.0
25.0
ppm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7.047
7.027
6.931
6.910
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2.650
2.637
2.629
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2.593
2.582
2.514
2.507
2.491
2.474
2.458
2.436
2.426
2.399
Cl
N
O
SMe
Ts
6m
8.0
7.5
7.0
ppm
3.2
3.0
2.8
2.6
ppm
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1.000
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1.036
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1.049
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1.0
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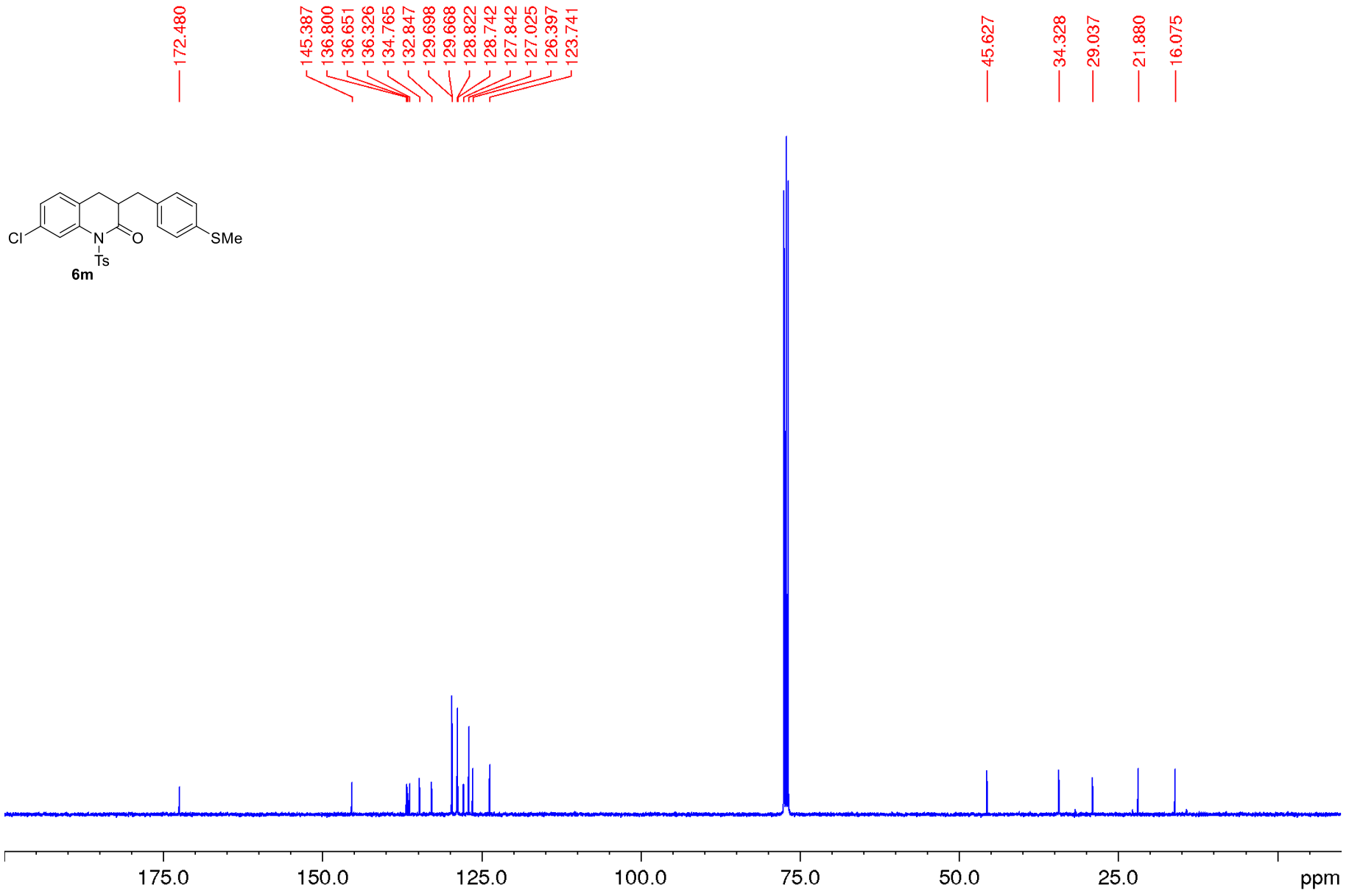
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SMe
Ts
6m
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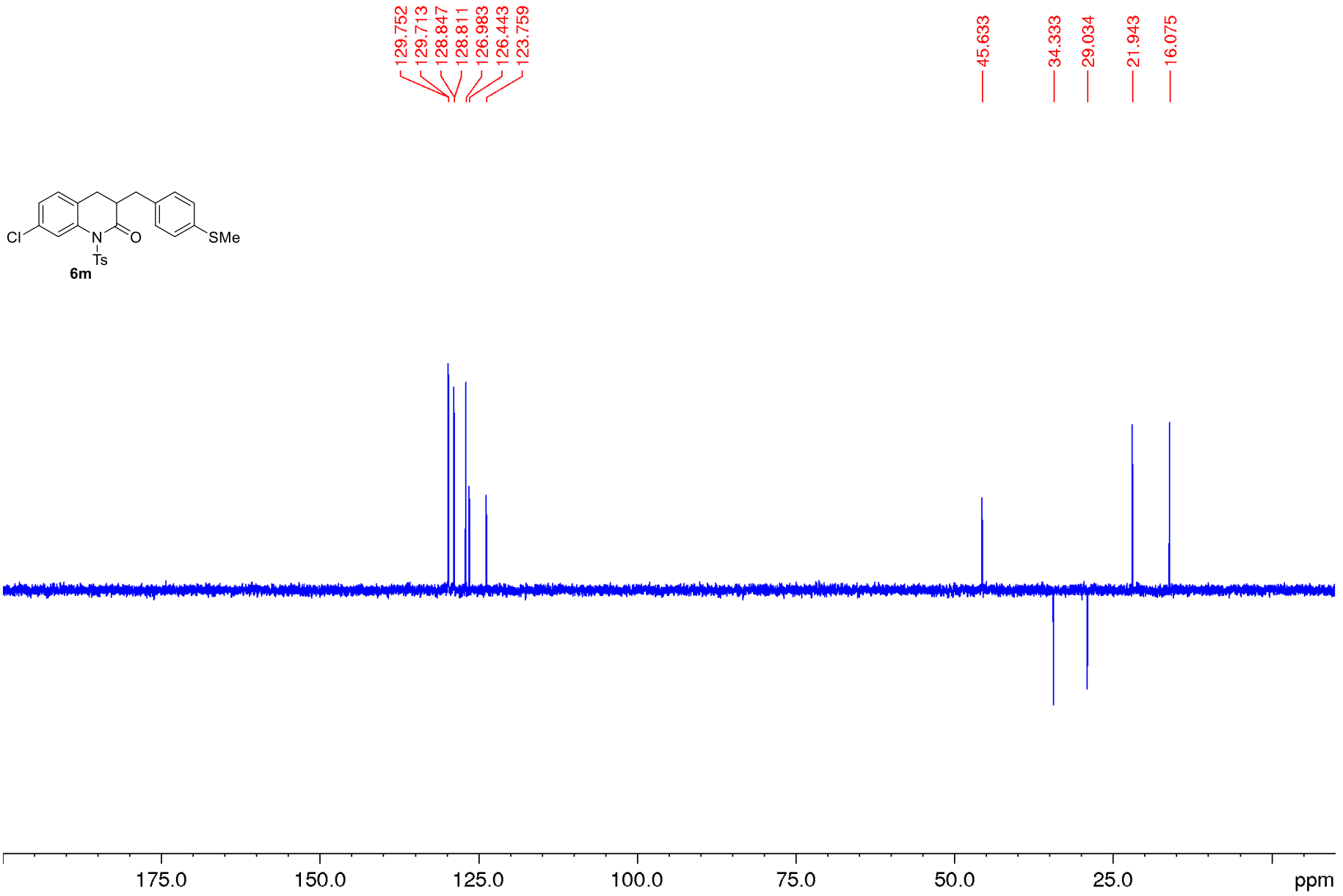
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Cl
N
O
SMe
Ts
6m
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100.0
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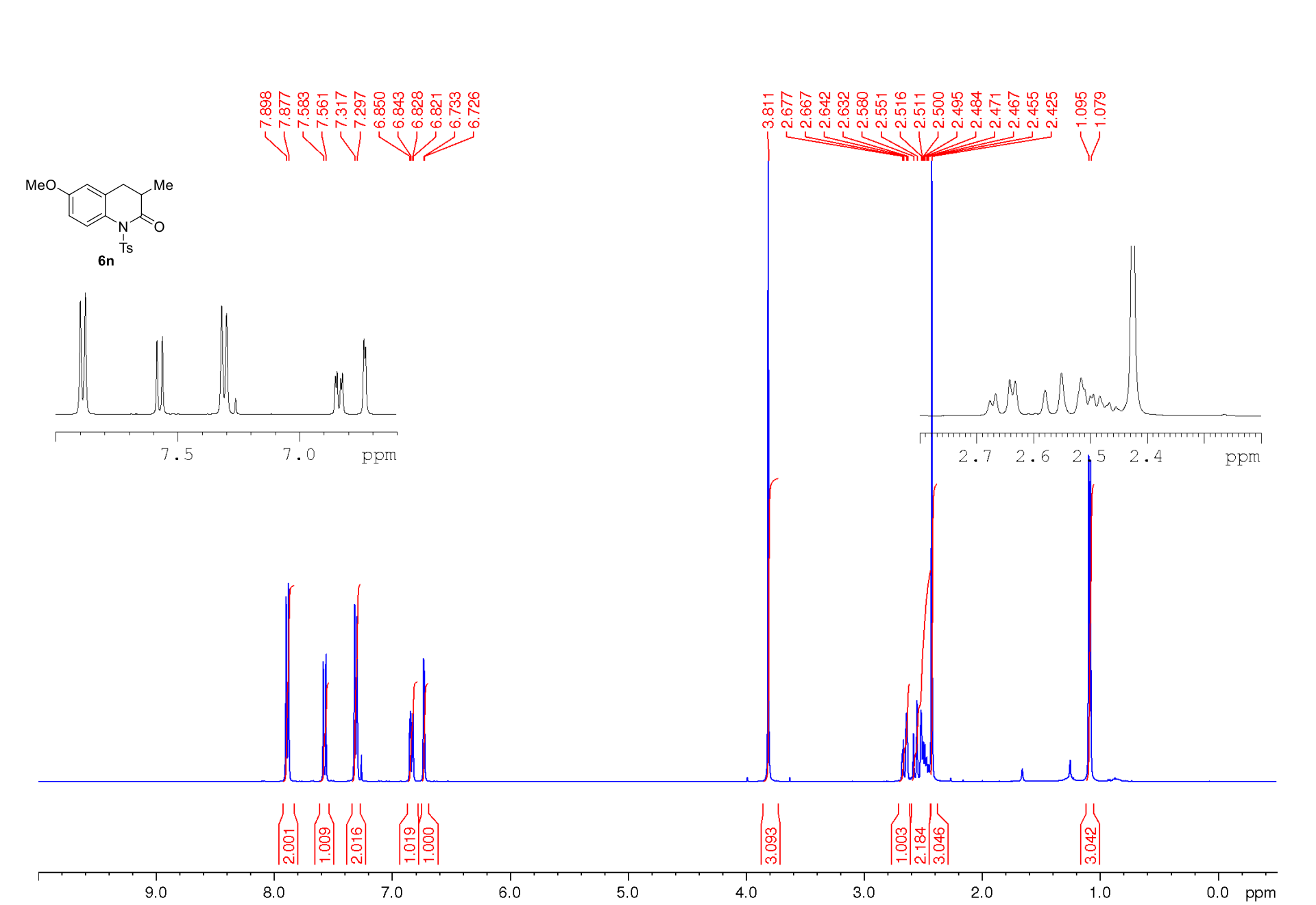
50.0
25.0
ppm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6.726
3.811
2.677
2.667
2.642
2.632
2.580
2.551
2.516
2.511
2.500
2.495
2.484
2.471
2.467
2.455
2.425
1.095
1.079
MeO
Me
N
O
Ts
6n
7.5
7.0
ppm
2.7
2.6
2.5
2.4
ppm
2.001
1.009
2.016
1.019
1.000
3.093
1.003
2.184
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1.0
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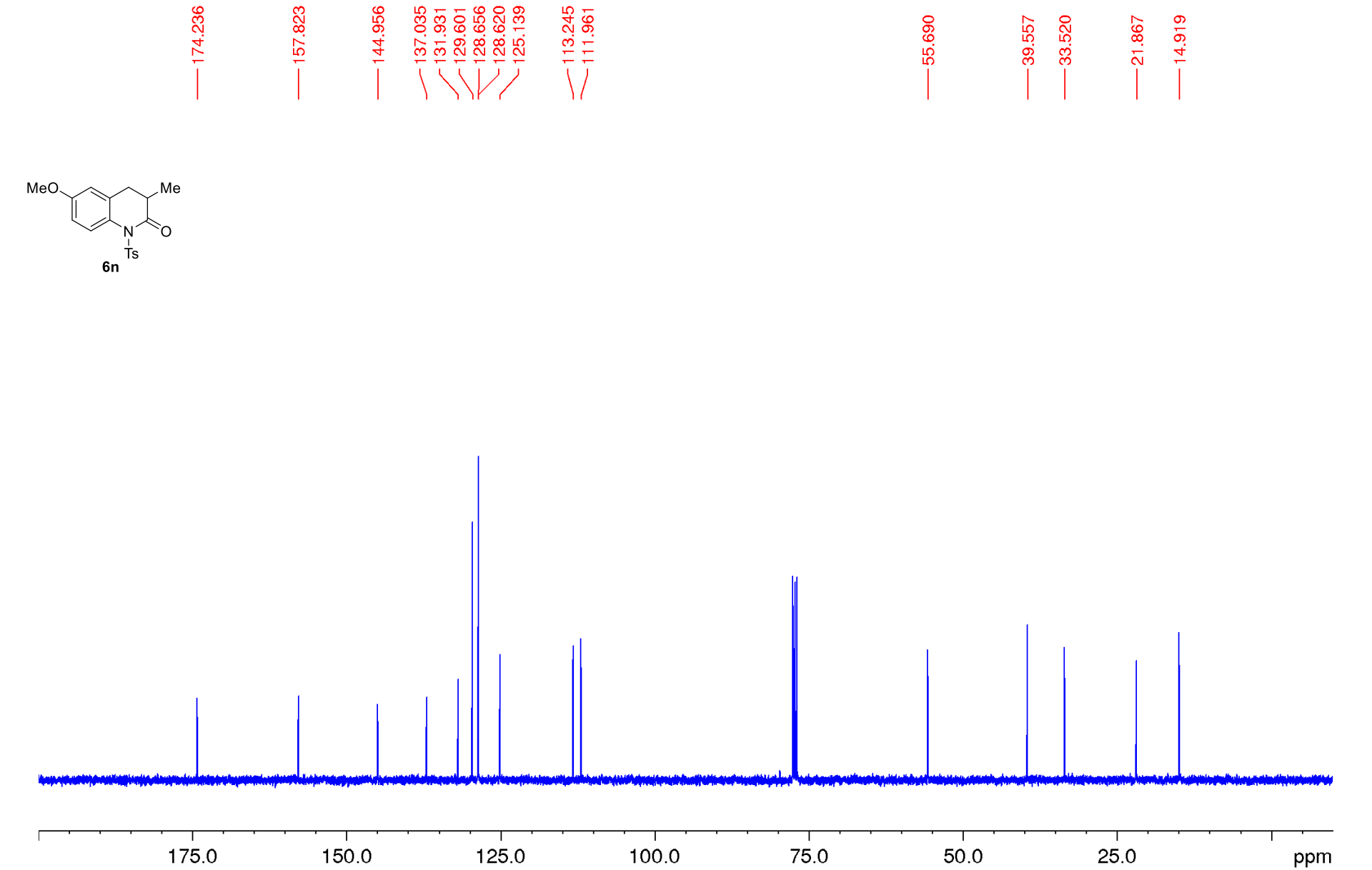
ppm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144.956
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128.656
128.620
125.139
113.245
111.961
55.690
39.557
33.520
21.867
14.919
MeO
Me
N
O
Ts
6n
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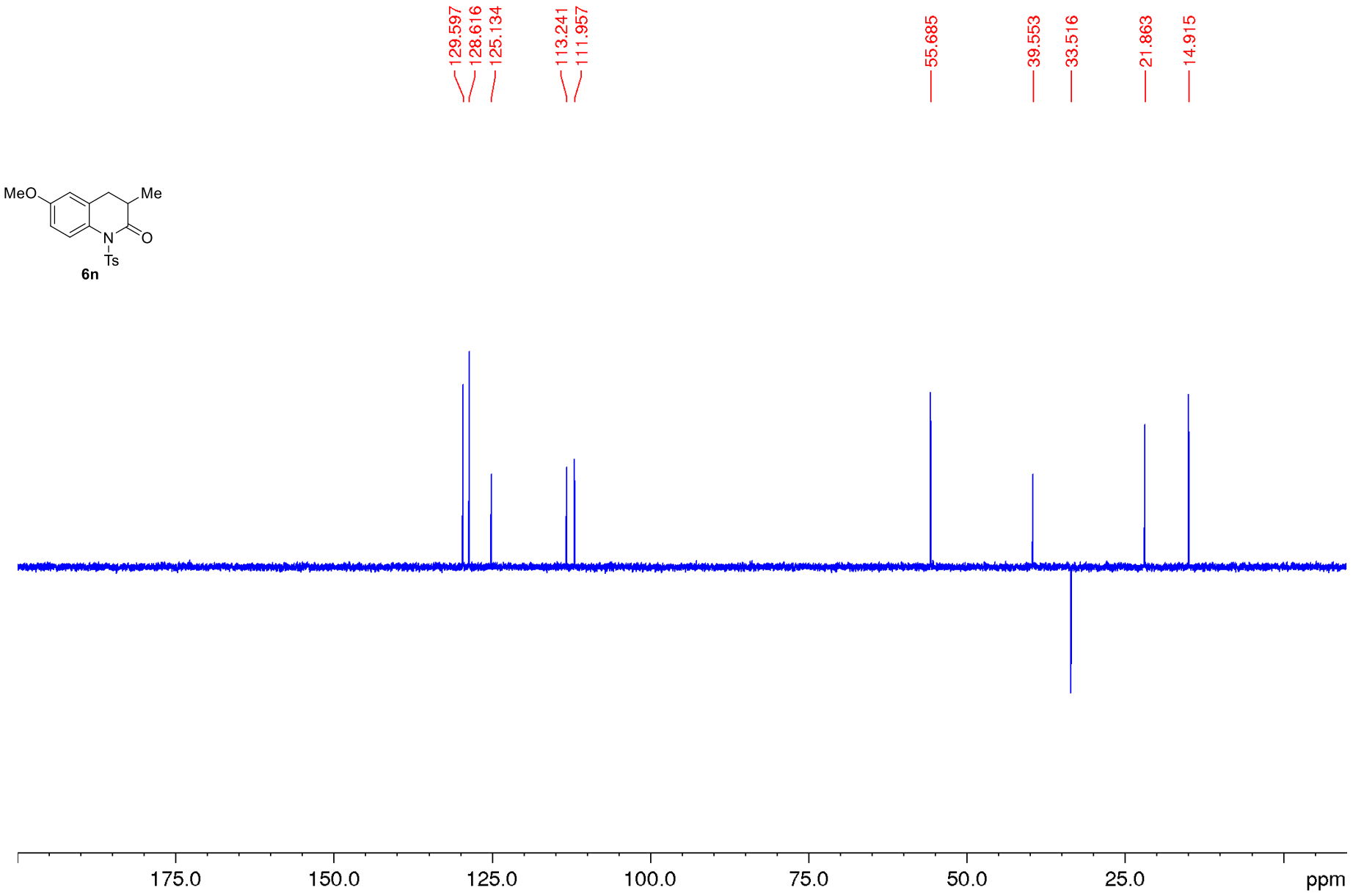
125.0
100.0
75.0
50.0
25.0
ppm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111.957
55.685
39.553
33.516
21.863
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Me
N
O
Ts
6n
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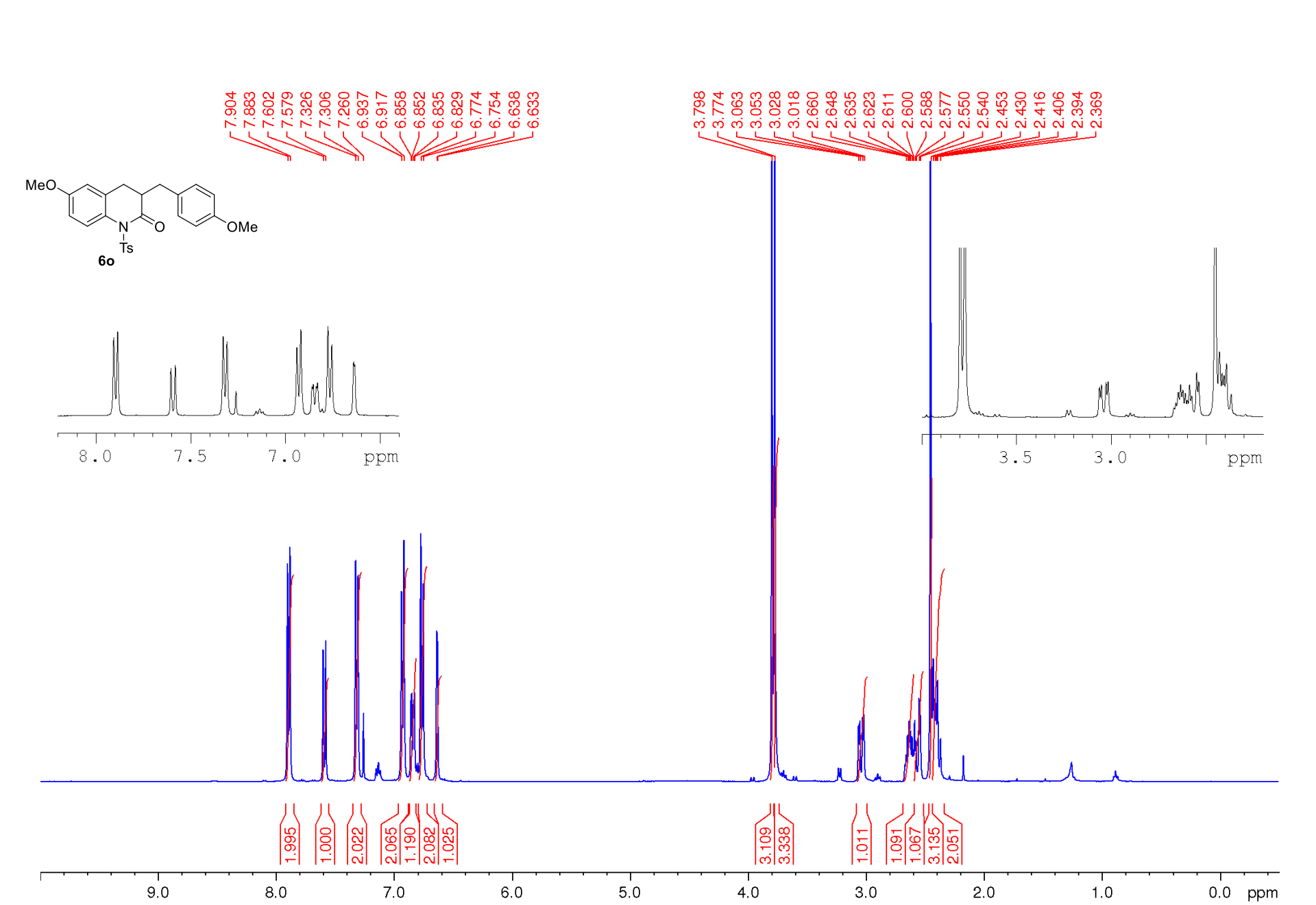
100.0
75.0
50.0
25.0
ppm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7.260
6.937
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6.835
6.829
6.774
6.754
6.638
6.633
3.798
3.774
3.063
3.053
3.028
3.018
2.660
2.648
2.635
2.623
2.611
2.600
2.588
2.577
2.550
2.540
2.453
2.430
2.416
2.406
2.394
2.369
MeO
OMe
N
O
Ts
6o
8.0
7.5
7.0
ppm
3.5
3.0
ppm
1.995
1.000
2.022
2.065
1.190
2.082
1.025
3.109
3.338
1.011
1.091
1.067
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3.0
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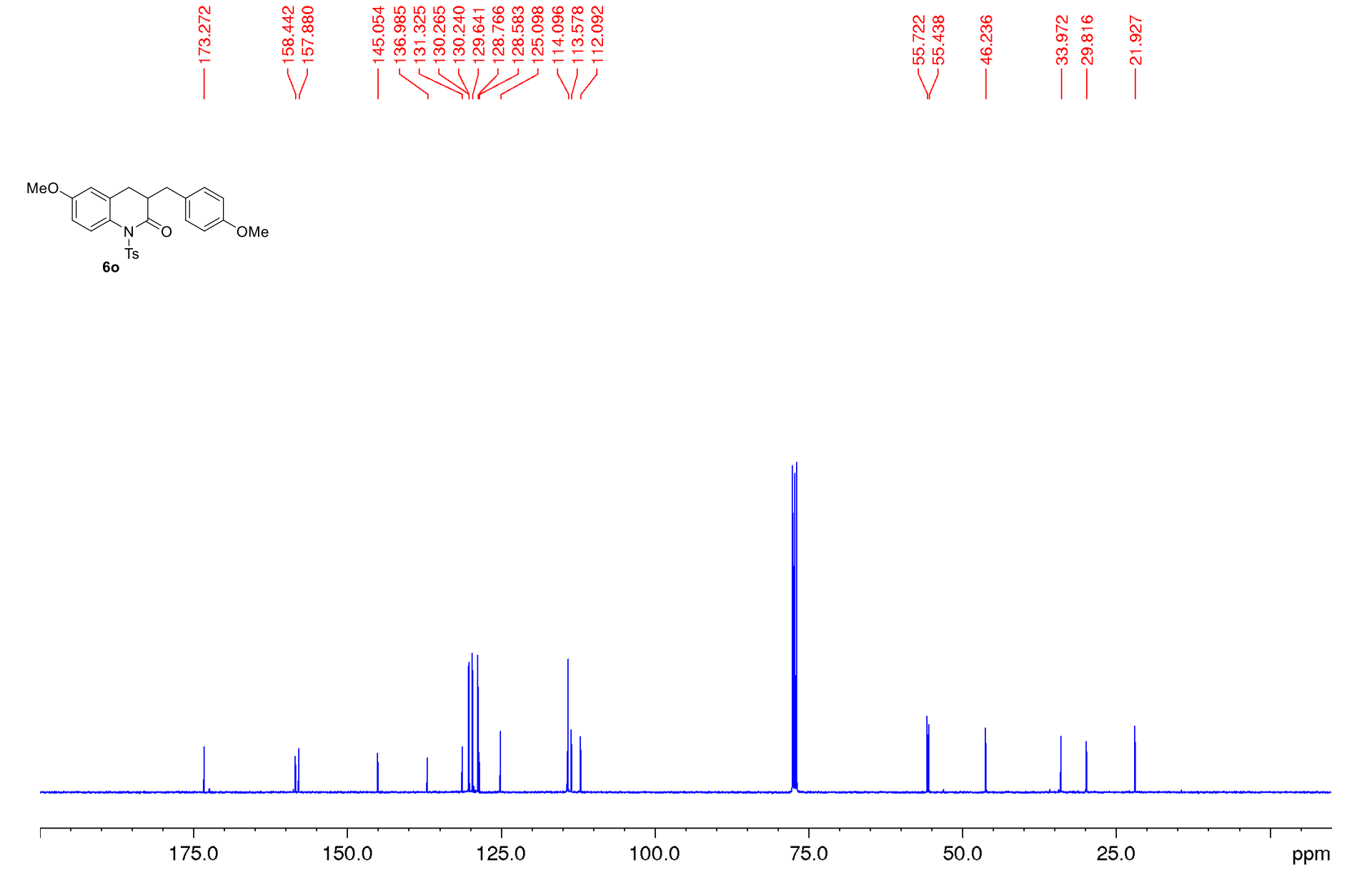
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125.098
114.096
113.578
112.092
55.722
55.438
46.236
33.972
29.816
21.927
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OMe
N
O
Ts
6o
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100.0
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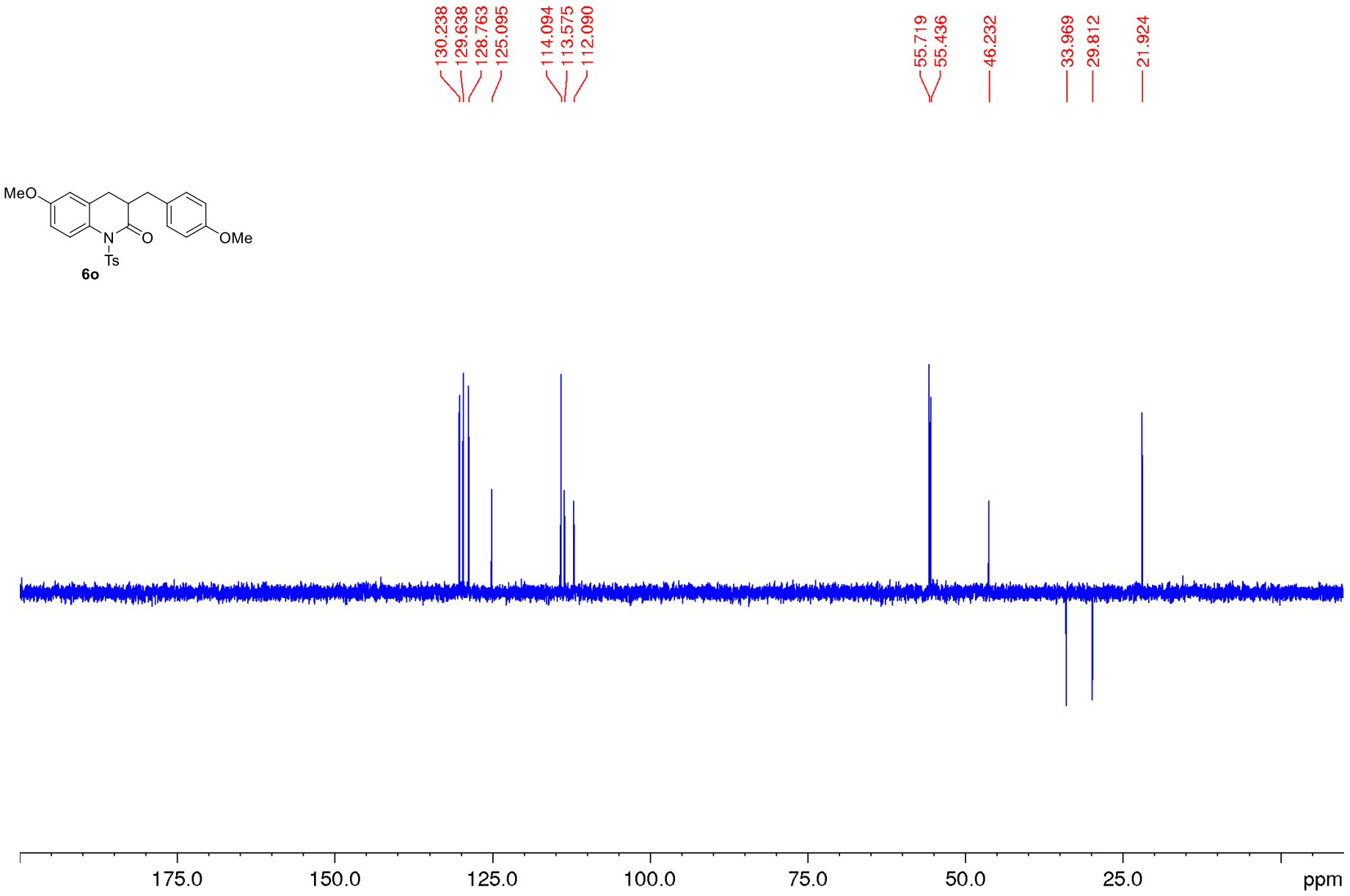
50.0
25.0
ppm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46.232
33.969
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21.924
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OMe
N
O
Ts
6o
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100.0
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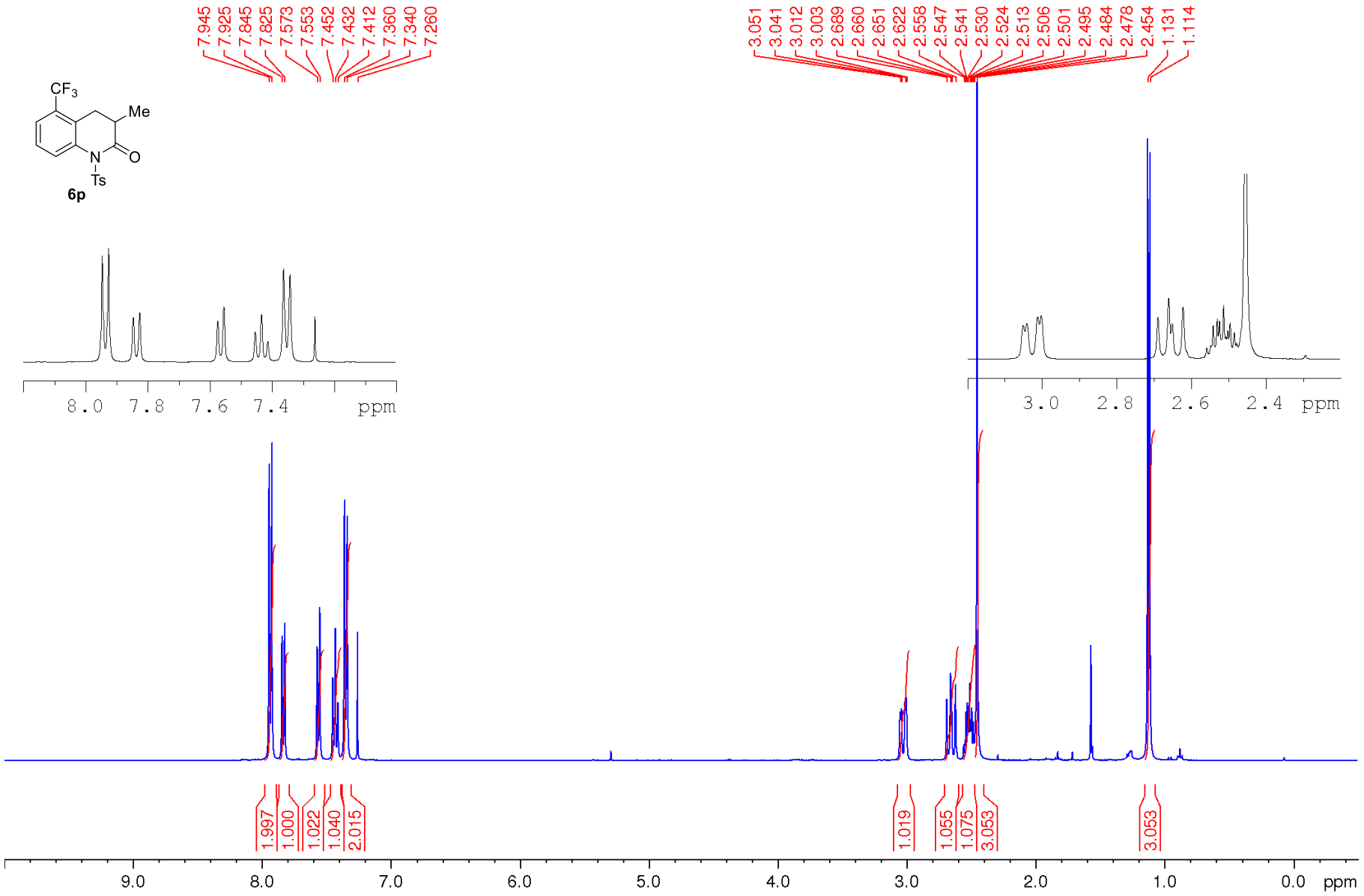
50.0
25.0
ppm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7.452
7.432
7.412
7.360
7.340
7.260
3.051
3.041
3.012
3.003
2.689
2.660
2.651
2.622
2.558
2.547
2.541
2.530
2.524
2.513
2.506
2.501
2.495
2.484
2.478
2.454
1.131
1.114
CF3
Me
N
O
Ts
6p
8.0
7.8
7.6
7.4
ppm
3.0
2.8
2.6
2.4
ppm
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1.000
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1.040
2.015
1.019
1.055
1.075
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8.0
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3.0
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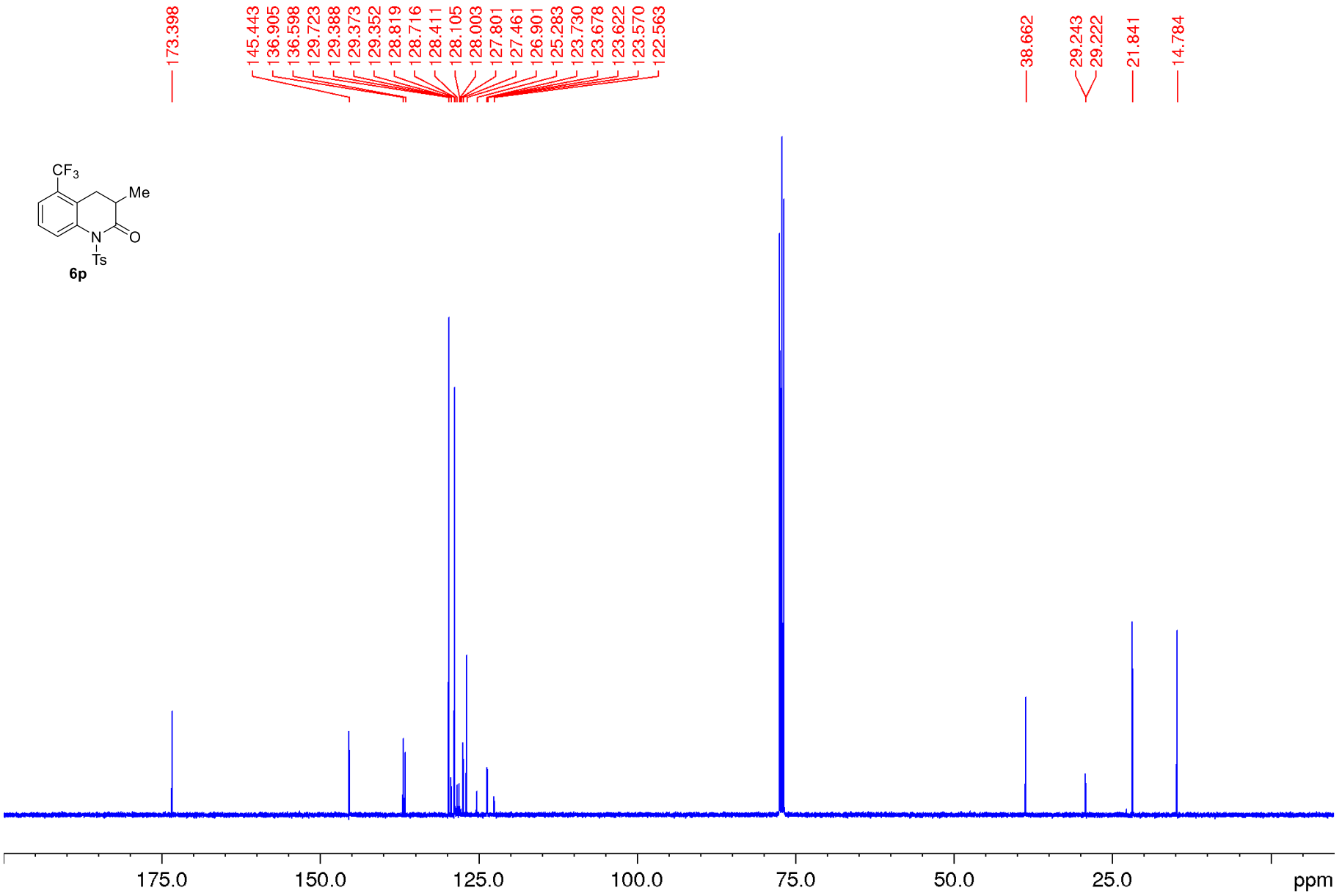
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126.901
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29.243
29.222
21.841
14.784
CF3
Me
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O
Ts
6p
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50.0
25.0
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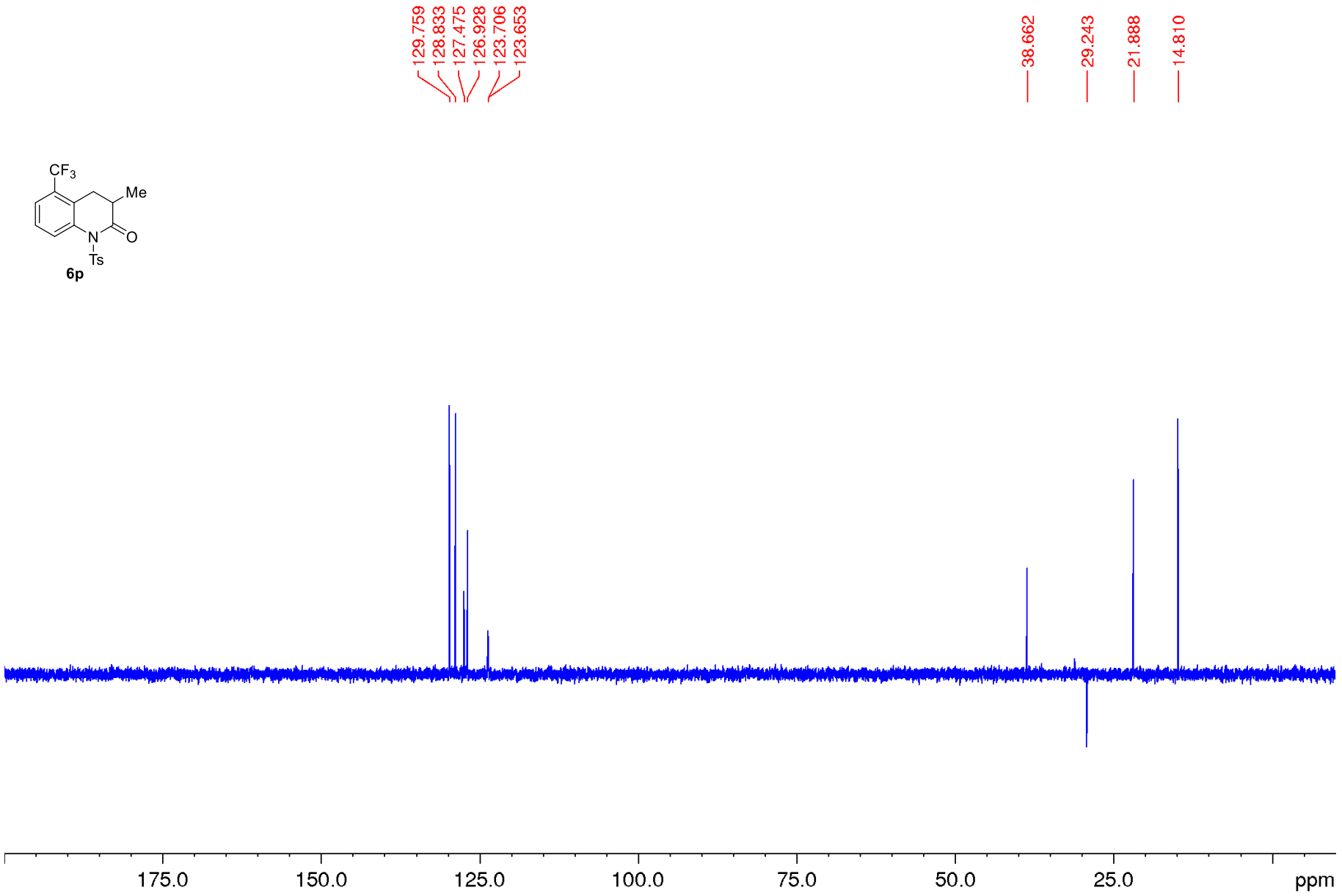
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29.243
21.888
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O
Ts
6p
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100.0
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50.0
25.0
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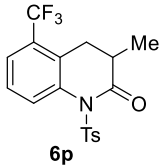
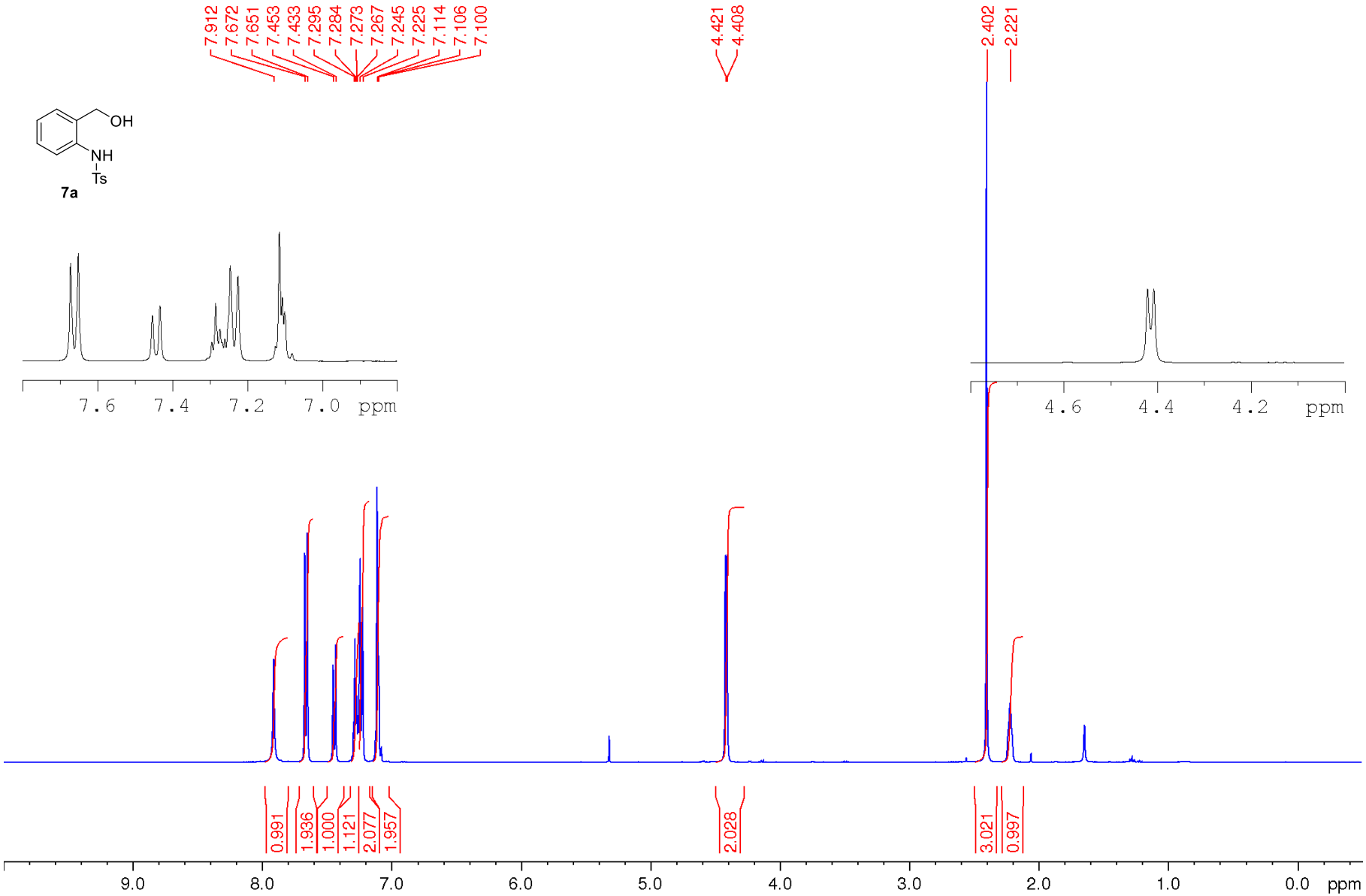


6p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7.225
7.114
7.106
7.100
4.421
4.408
2.402
2.221
OH
NH
Ts
7a
7.6
7.4
7.2
7.0
ppm
4.6
4.4
4.2
ppm
0.991
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1.000
1.121
2.077
1.957
2.028
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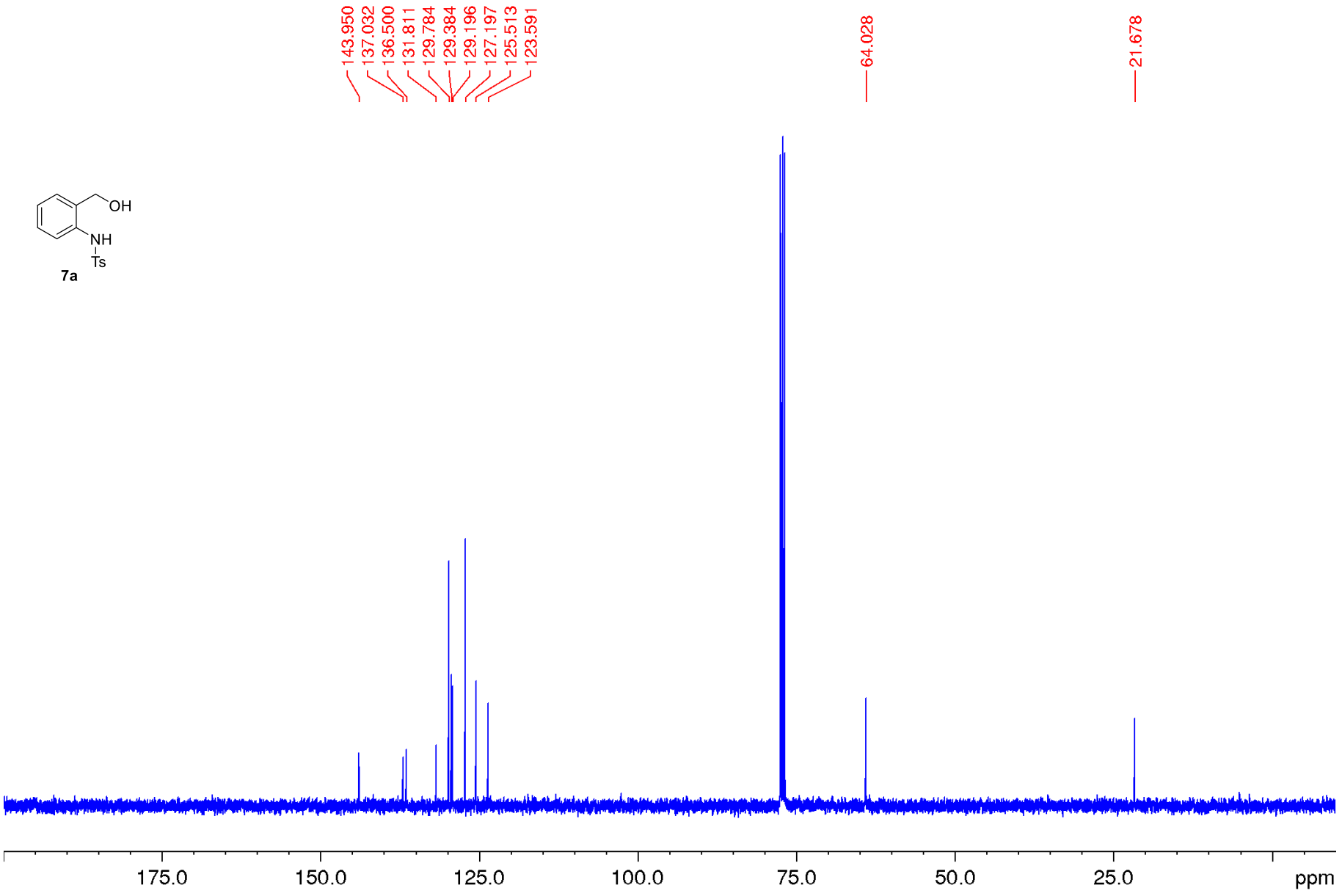
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Ts
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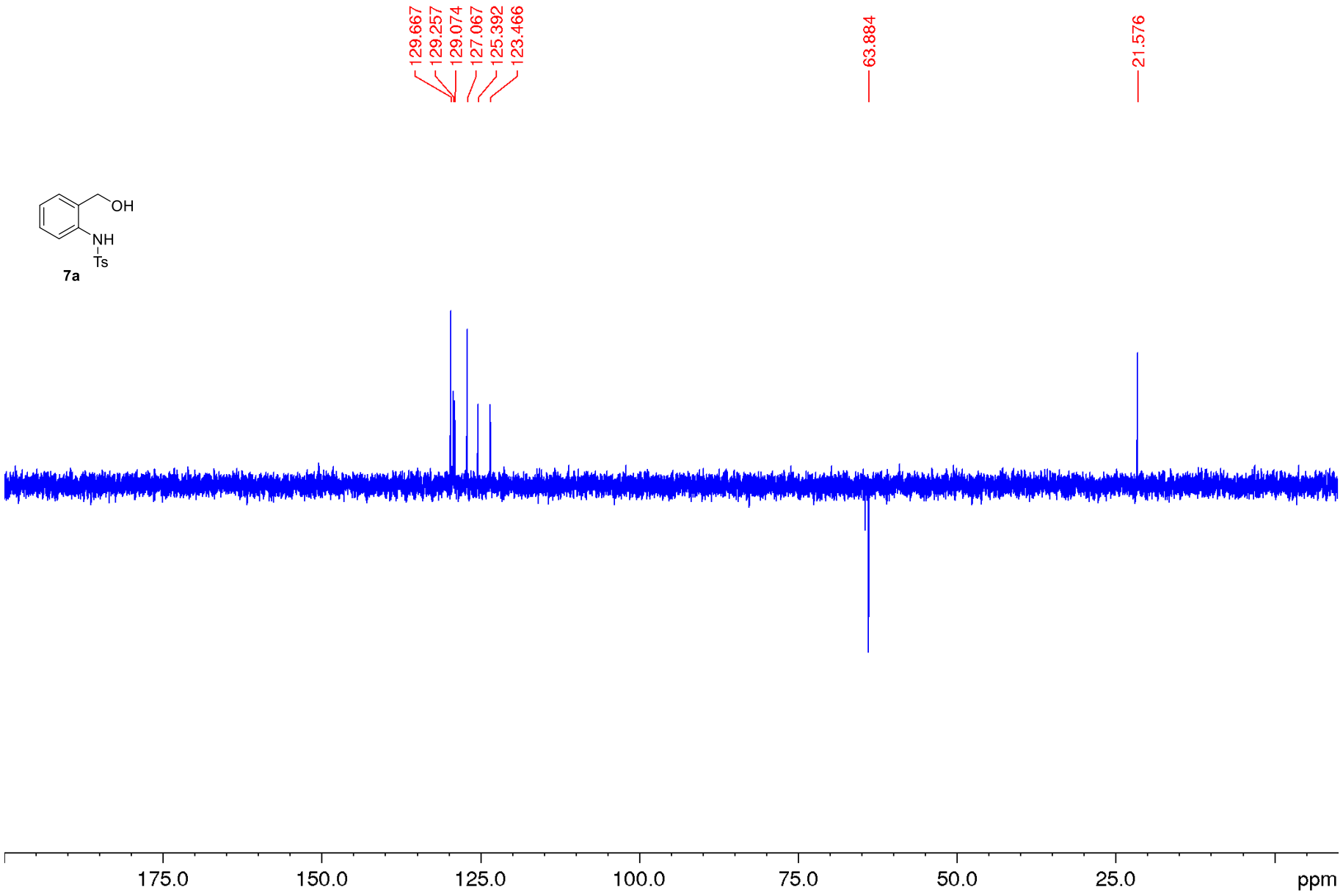
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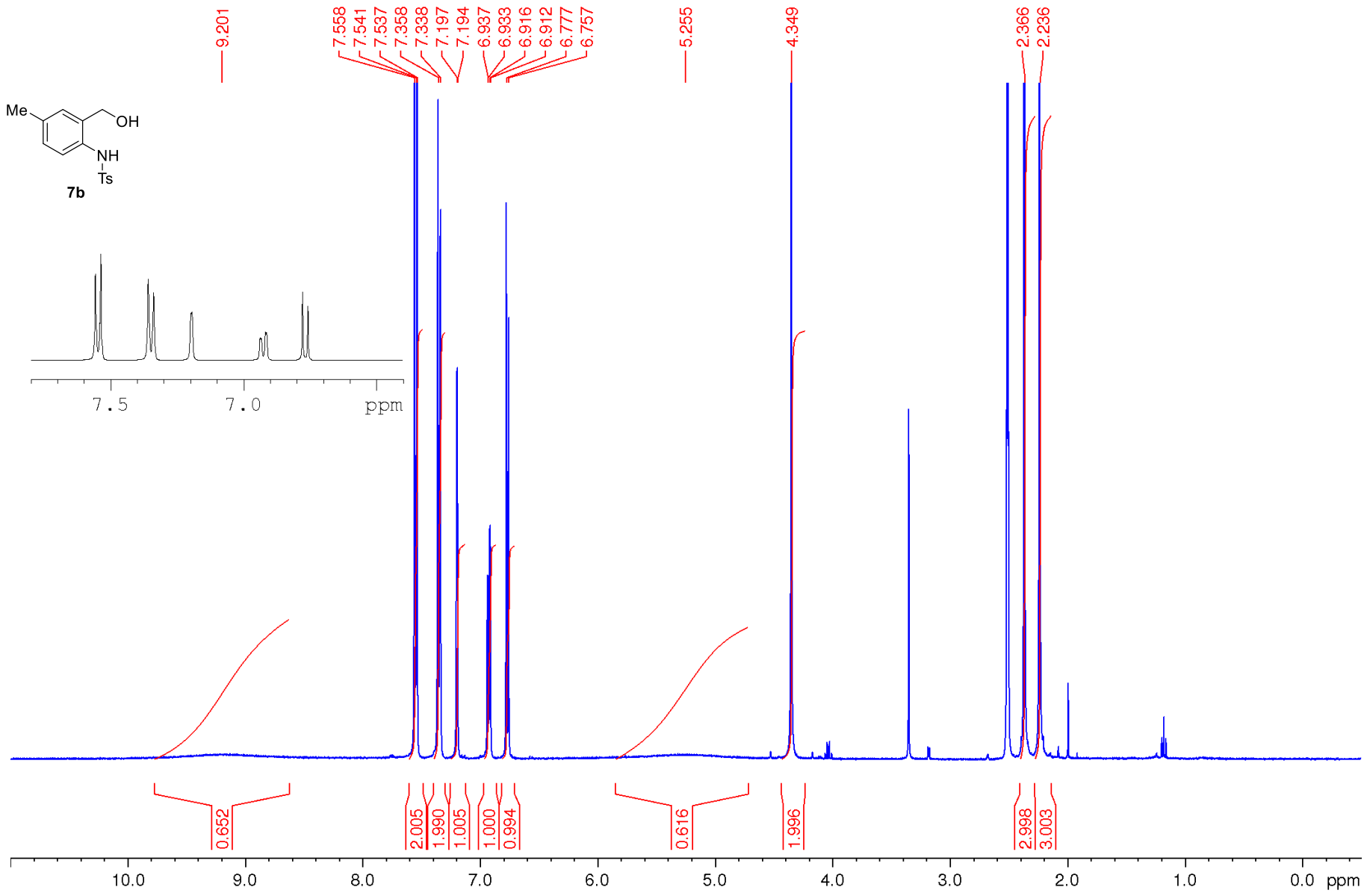
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7.194
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6.777
6.757
5.255
4.349
2.366
2.236
Me
OH
NH
Ts
7b
7.5
7.0
ppm
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1.005
1.000
0.994
0.616
1.996
2.998
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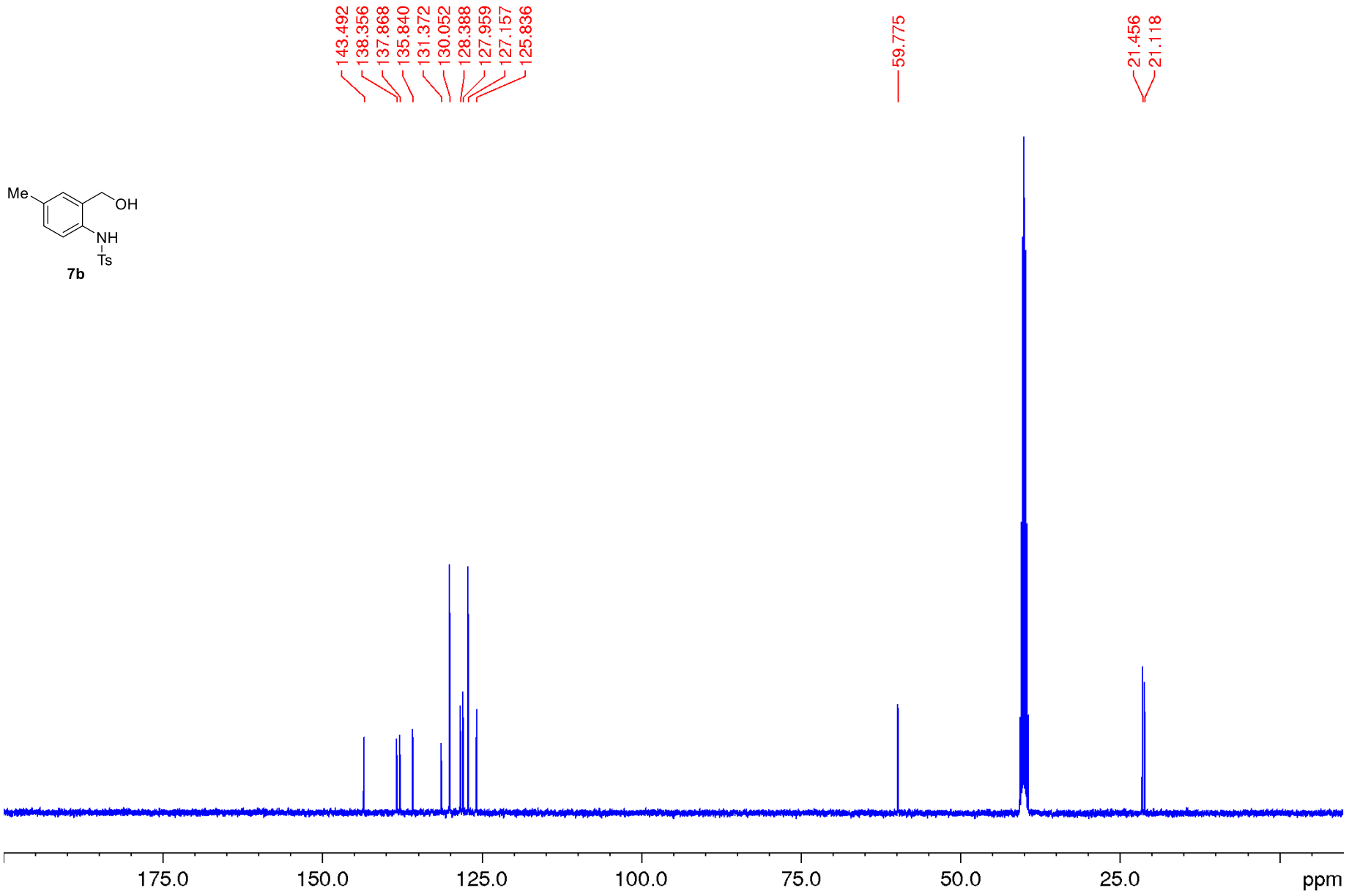
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21.456
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OH
NH
Ts
7b
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100.0
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50.0
25.0
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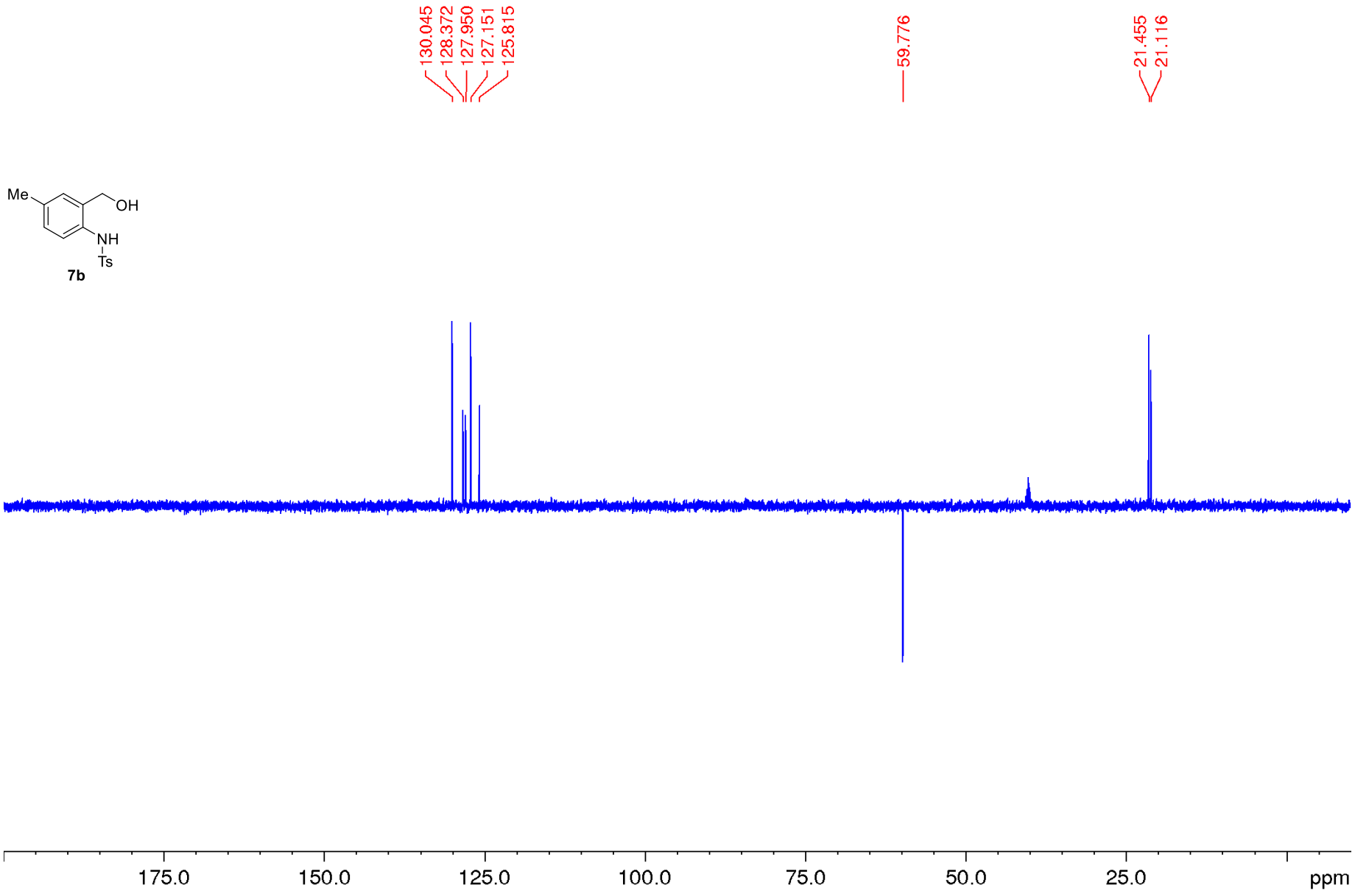
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Ts
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25.0
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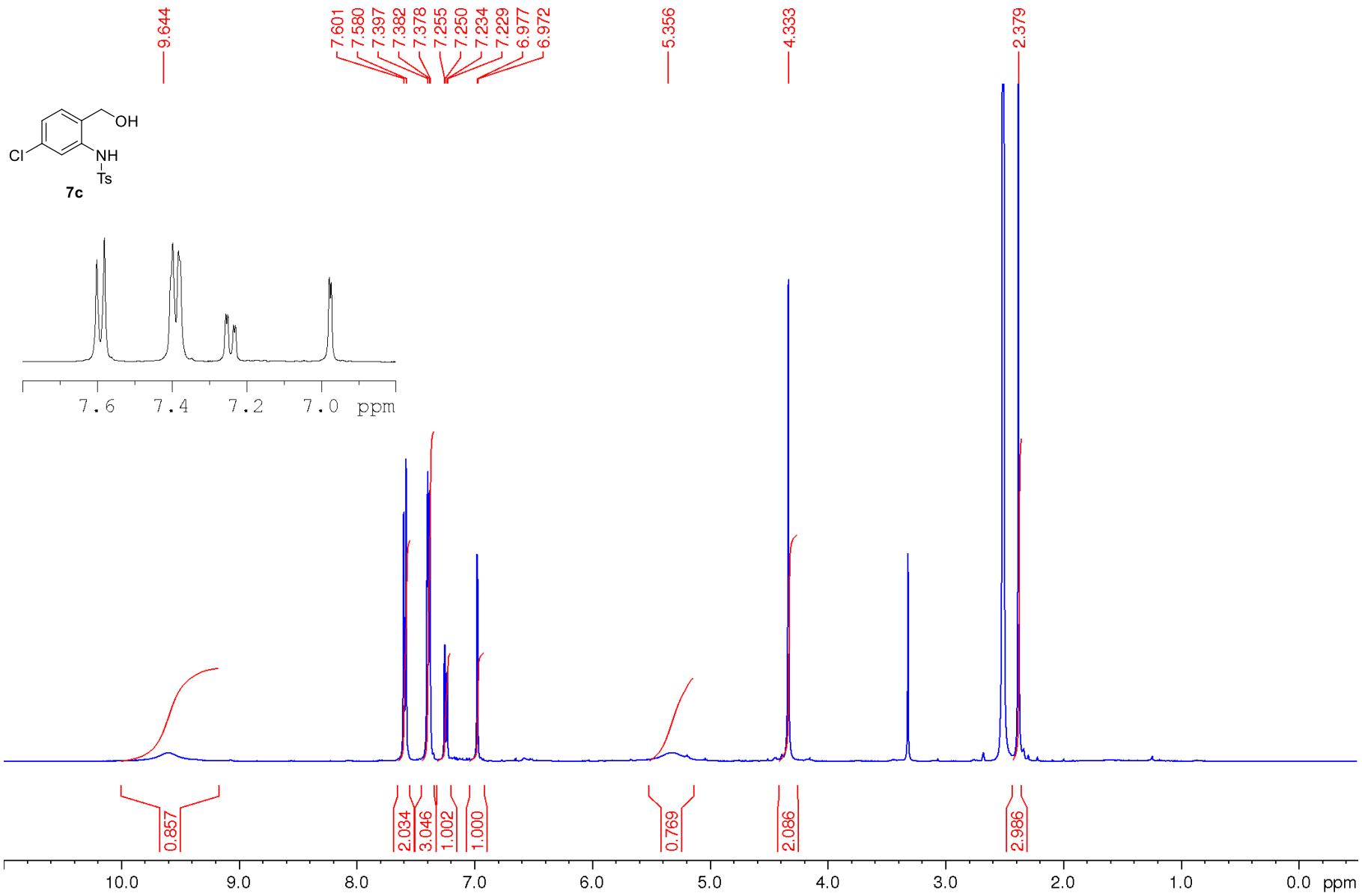
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7.229
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6.972
5.356
4.333
2.379
OH
Cl
NH
Ts
7c
7.6
7.4
7.2
7.0
ppm
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2.034
3.046
1.002
1.000
0.769
2.086
2.986
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4.0
3.0
2.0
1.0
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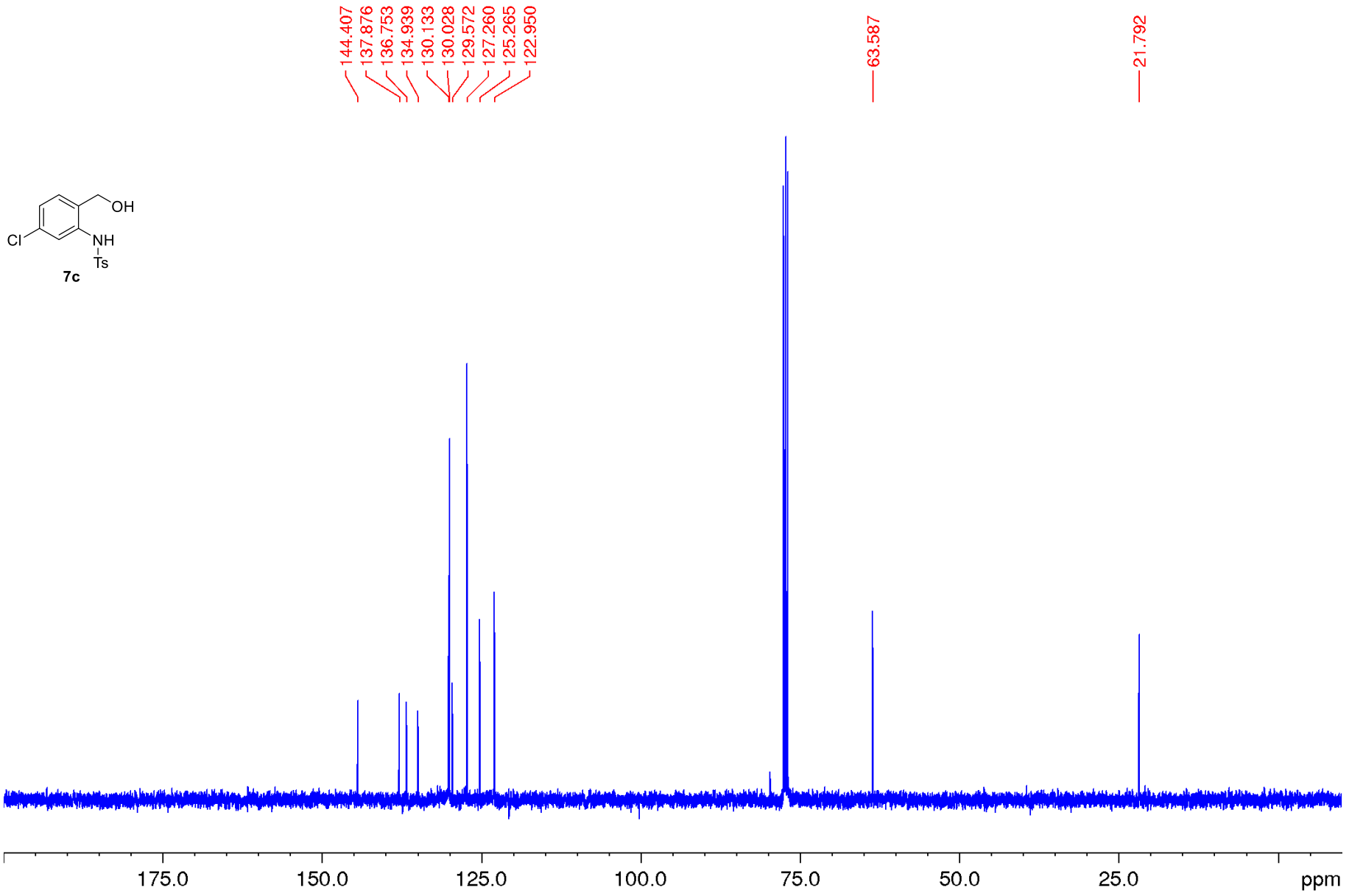
ppm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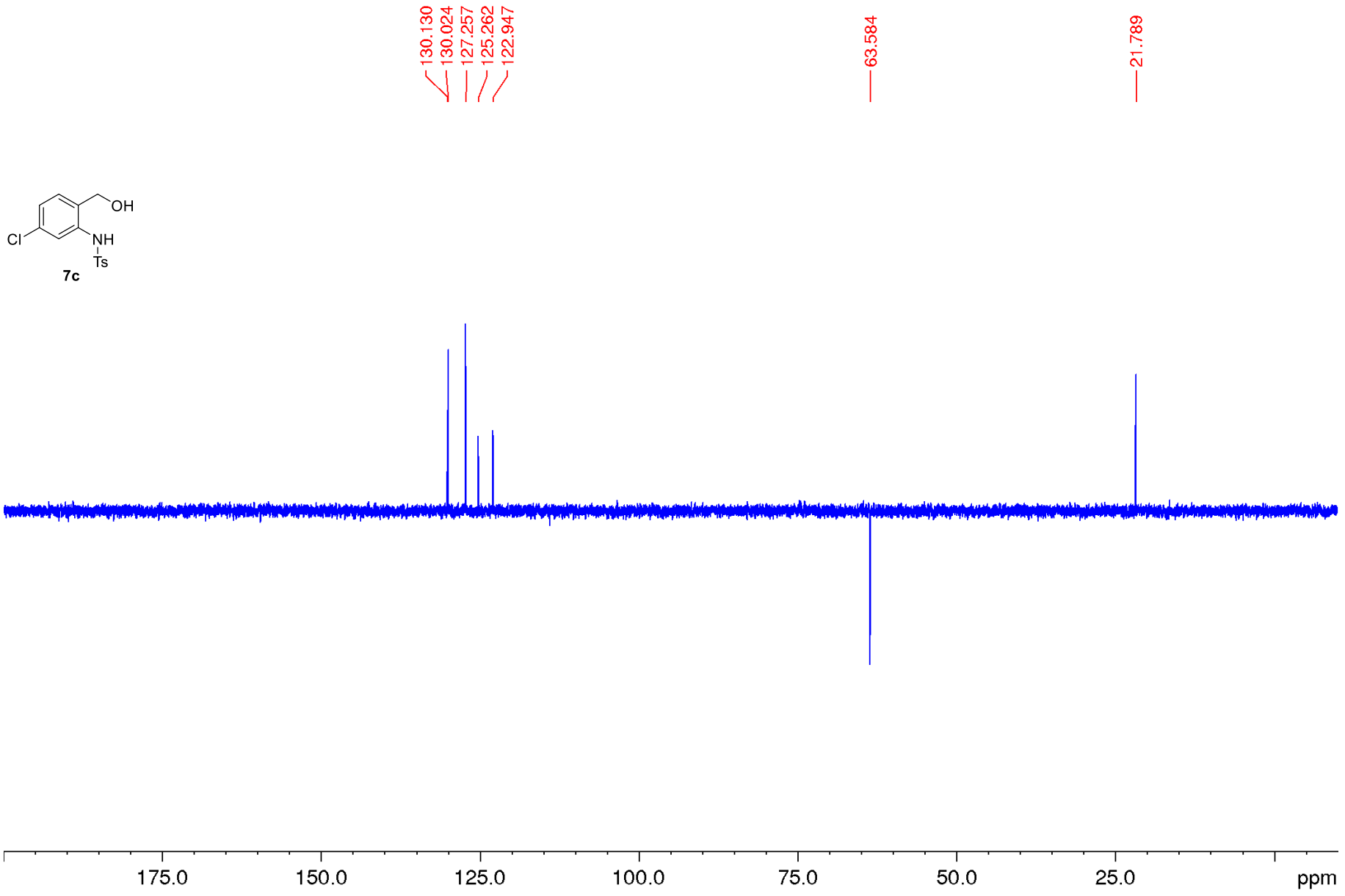
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NH
Ts
7c
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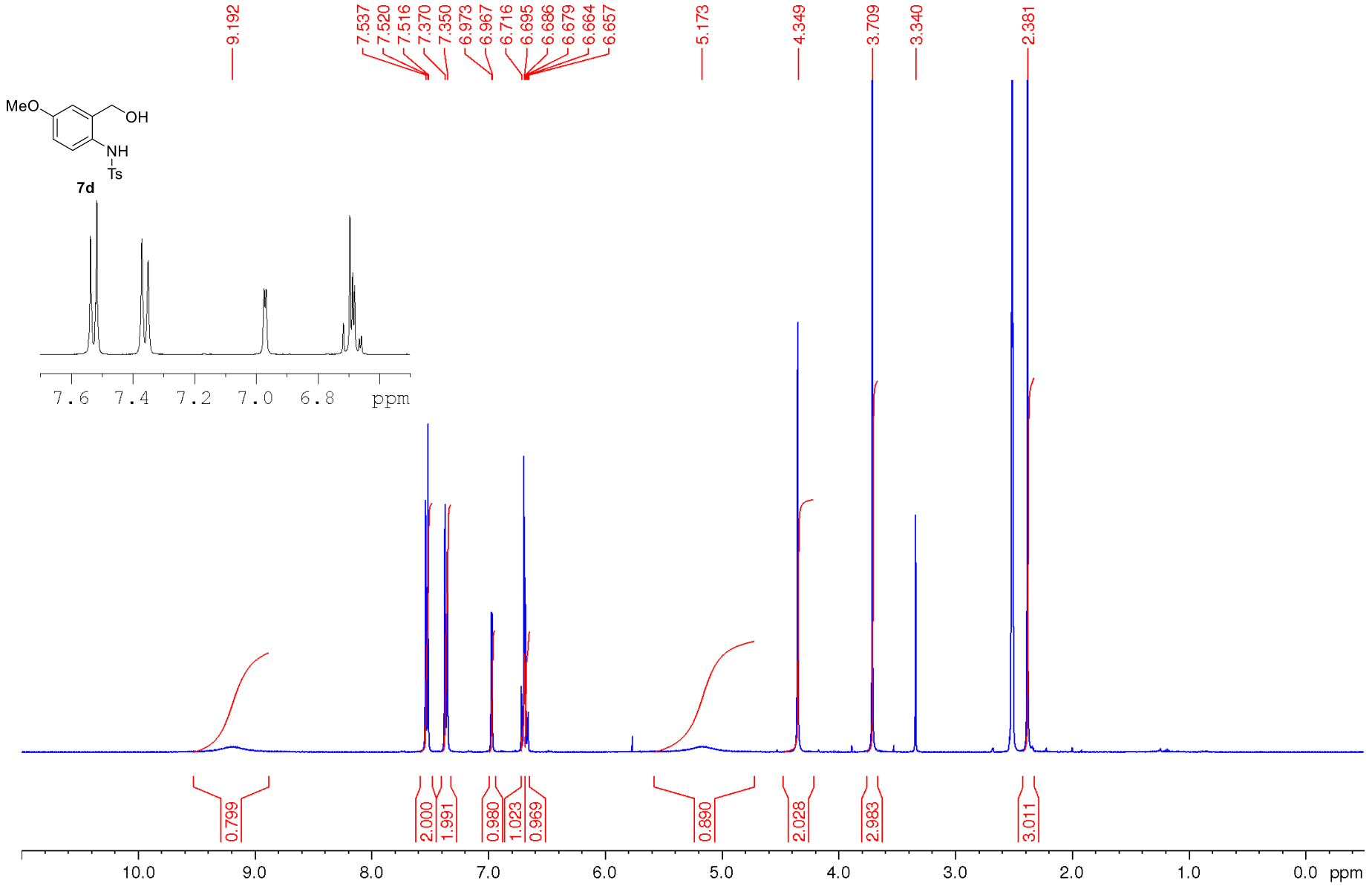
150.0
125.0
100.0
75.0
50.0
25.0
ppm


9.192
7.537
7.520
7.516
7.370
7.350
6.973
6.967
6.716
6.695
6.686
6.679
6.664
6.657
5.173
4.349
3.709
3.340
2.381
MeO
OH
NH
Ts
7d
7.6
7.4
7.2
7.0
6.8
ppm
0.799
2.000
1.991
0.980
1.023
0.969
0.890
2.028
2.983
3.011
10.0
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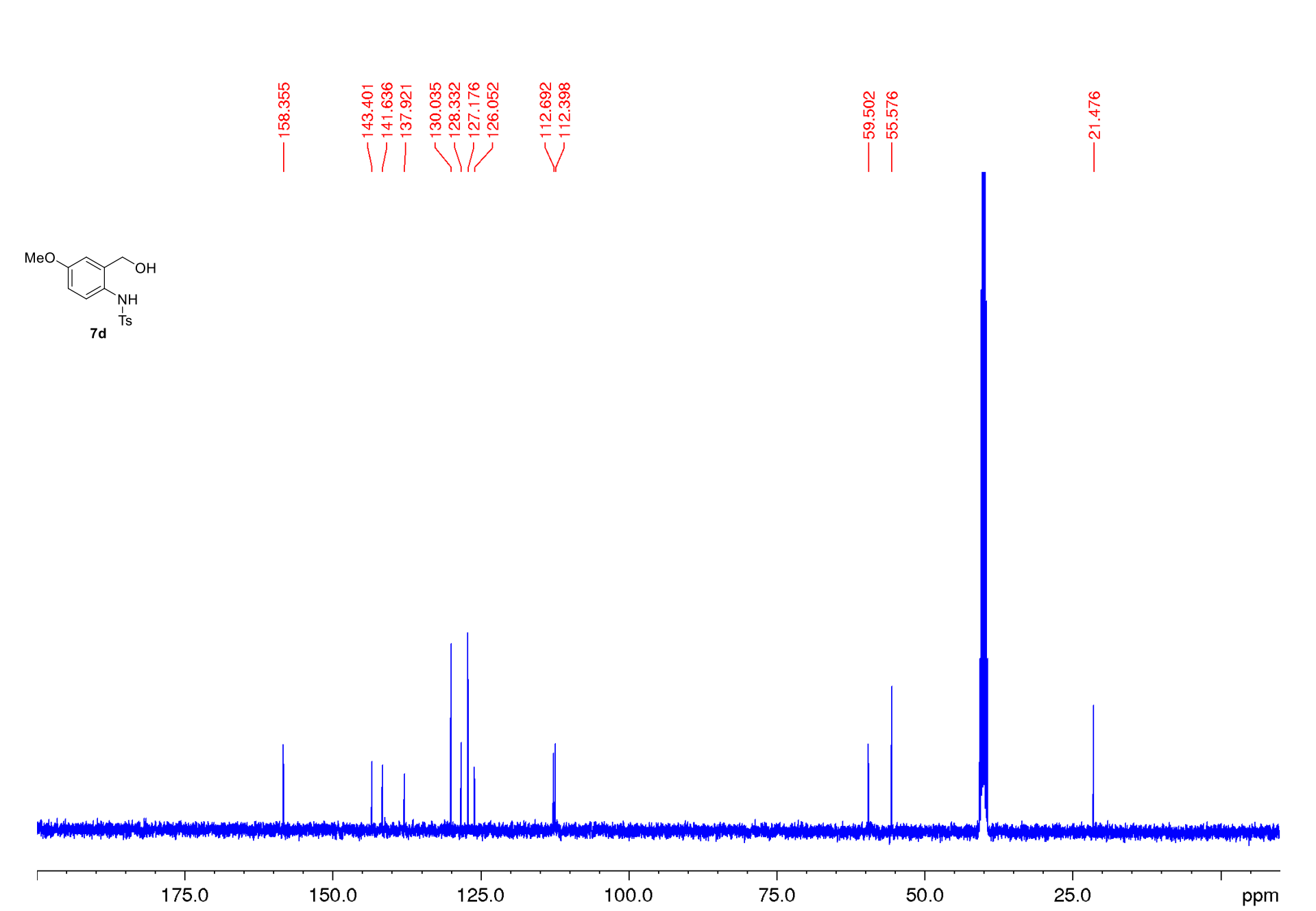
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm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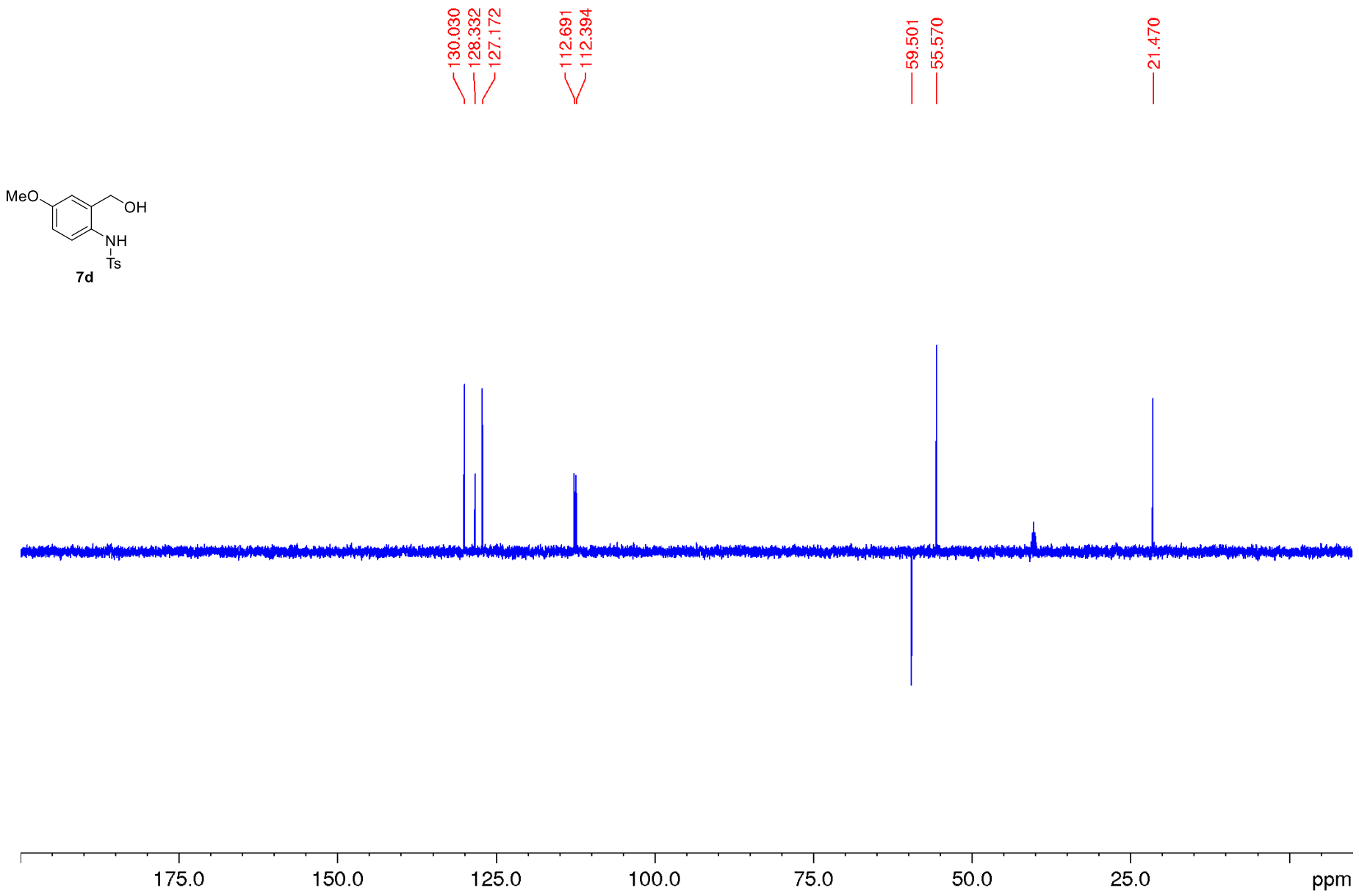
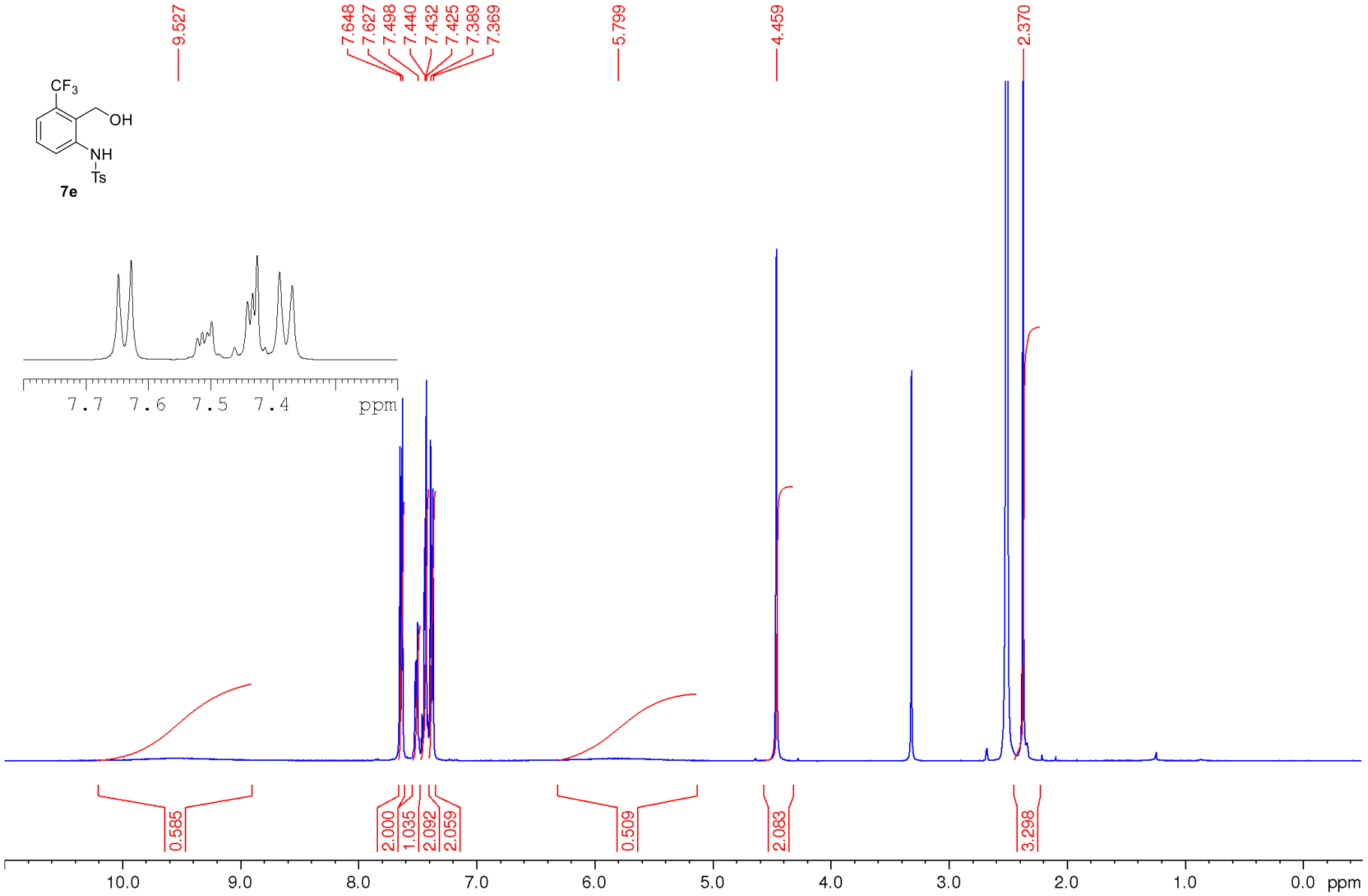
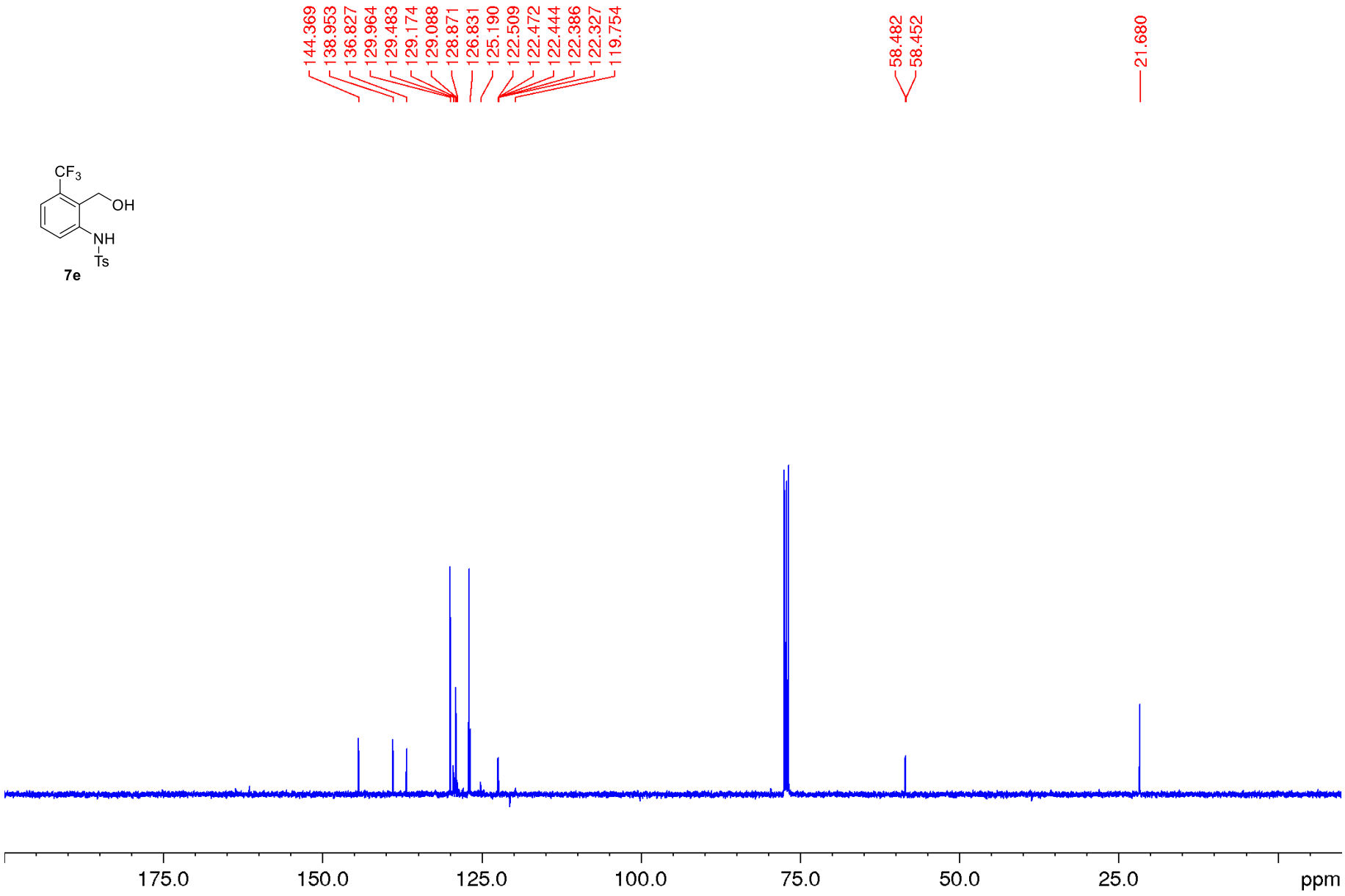
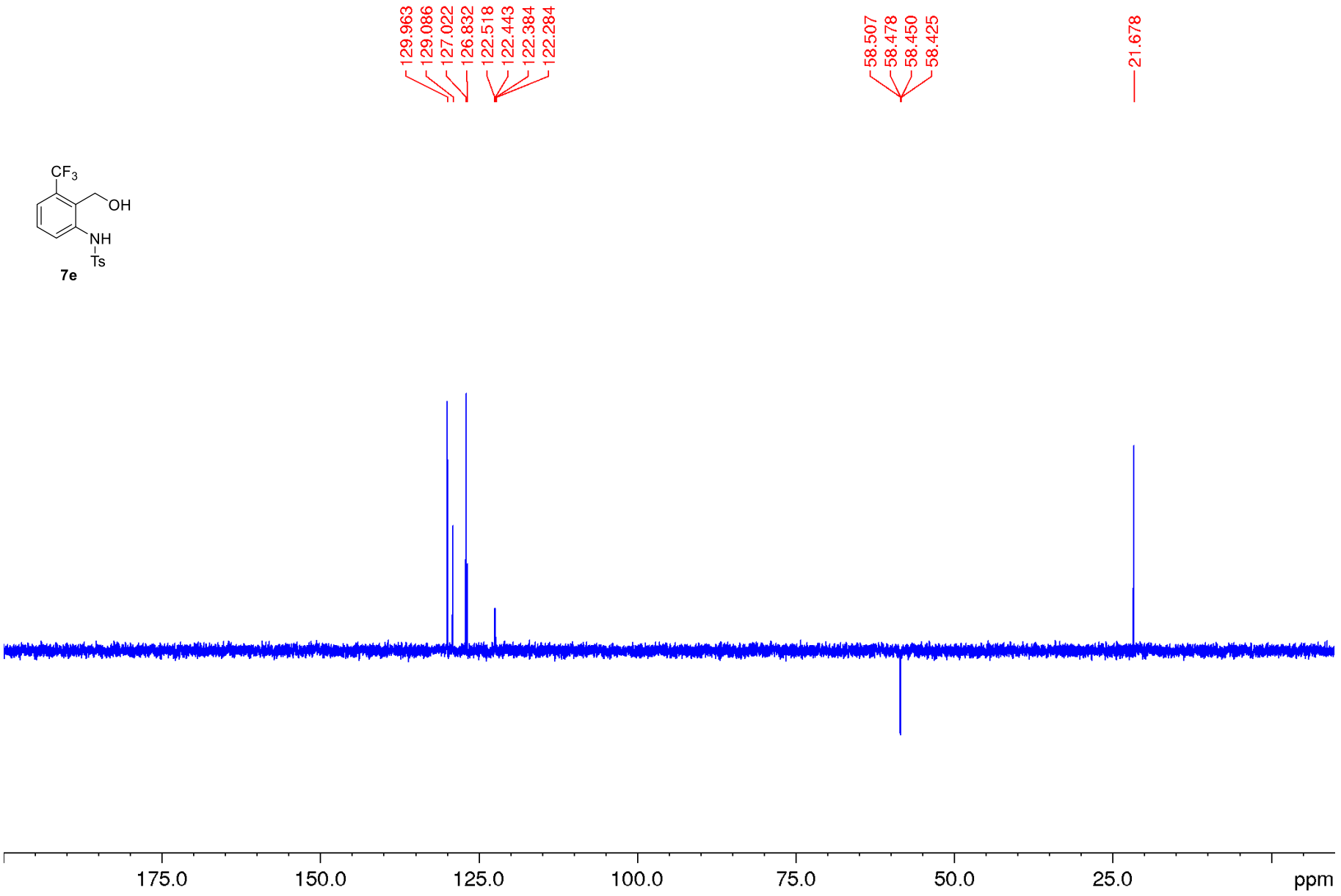
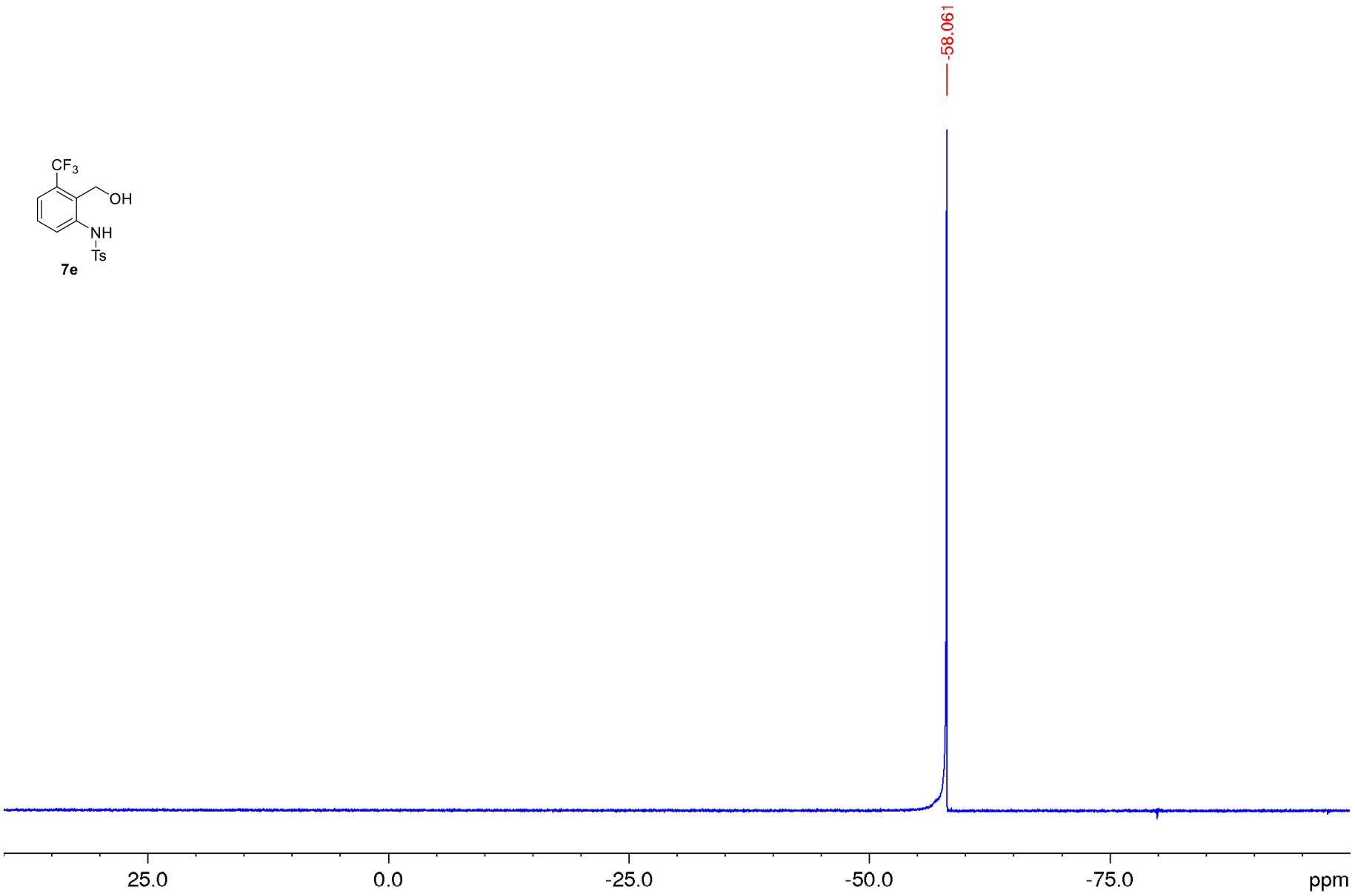
143.401
141.636
137.921
130.035
128.332
127.176
126.052
112.692
112.398
59.502
55.576
21.476
MeO
OH
NH
Ts
7d
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

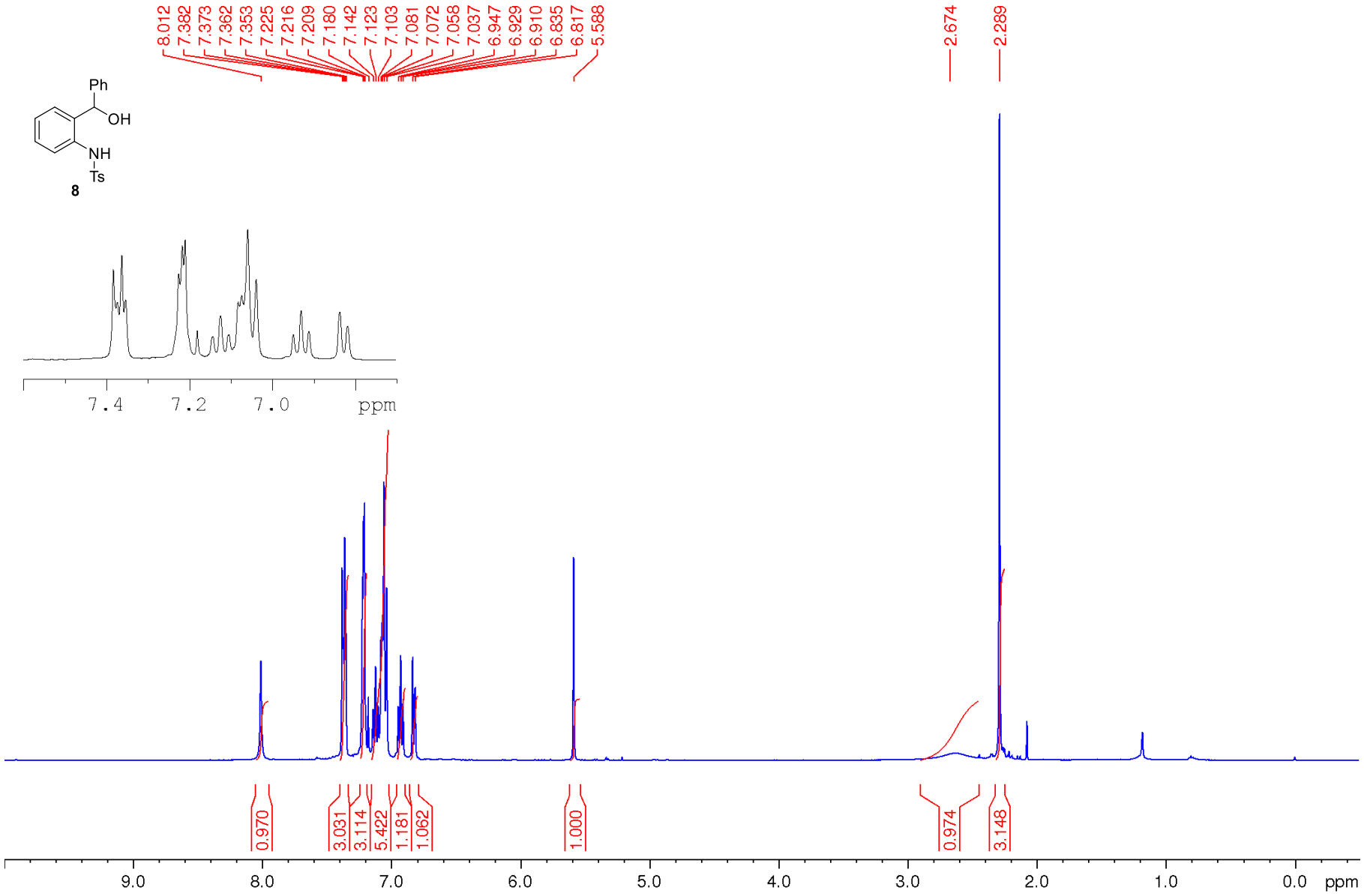

130.030
128.332
127.172
112.691
112.394
59.501
55.570
21.470
MeO
OH
NH
Ts
7d
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

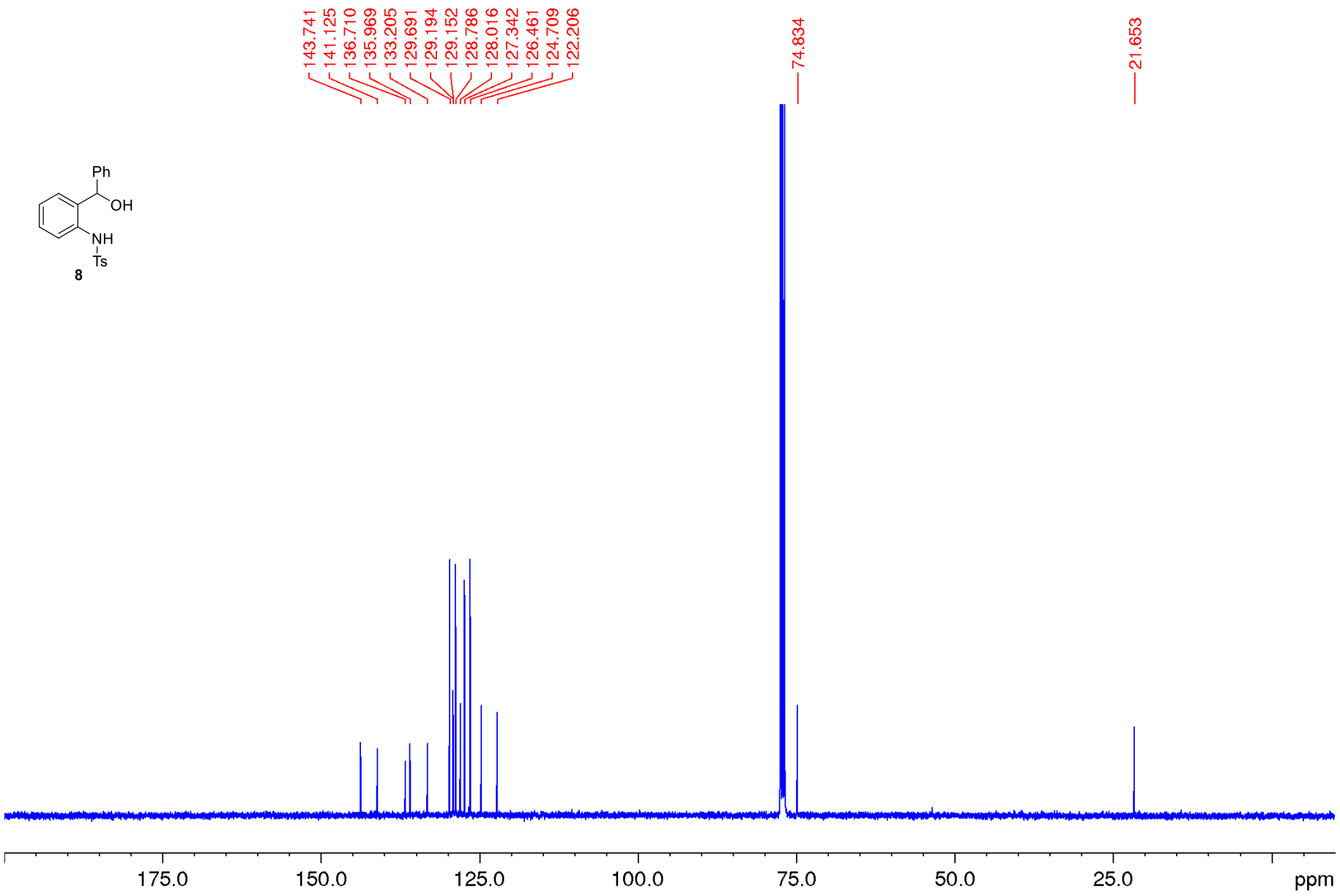

9.527
7.648
7.627
7.498
7.440
7.432
7.425
7.389
7.369
5.799
4.459
2.370
CF3
OH
NH
Ts
7e
7.7
7.6
7.5
7.4
ppm
0.585
2.000
1.035
2.092
2.059
0.509
2.083
3.298
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


144.369
138.953
136.827
129.964
129.483
129.174
129.088
128.871
126.831
125.190
122.509
122.472
122.444
122.386
122.327
119.754
58.482
58.452
21.680
CF3
OH
NH
Ts
7e
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


129.963
129.086
127.022
126.832
122.518
122.443
122.384
122.284
58.507
58.478
58.450
58.425
21.678
CF3
OH
NH
Ts
7e
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


-58.061
CF3
OH
NH
Ts
7e
25.0
0.0
-25.0
-50.0
-75.0
ppm


8.012
7.382
7.373
7.362
7.353
7.225
7.216
7.209
7.180
7.142
7.123
7.103
7.081
7.072
7.058
7.037
6.947
6.929
6.910
6.835
6.817
5.588
2.674
2.289
Ph
OH
NH
Ts
8
7.4
7.2
7.0
ppm
0.970
3.031
3.114
5.422
1.181
1.062
1.000
0.974
3.148
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm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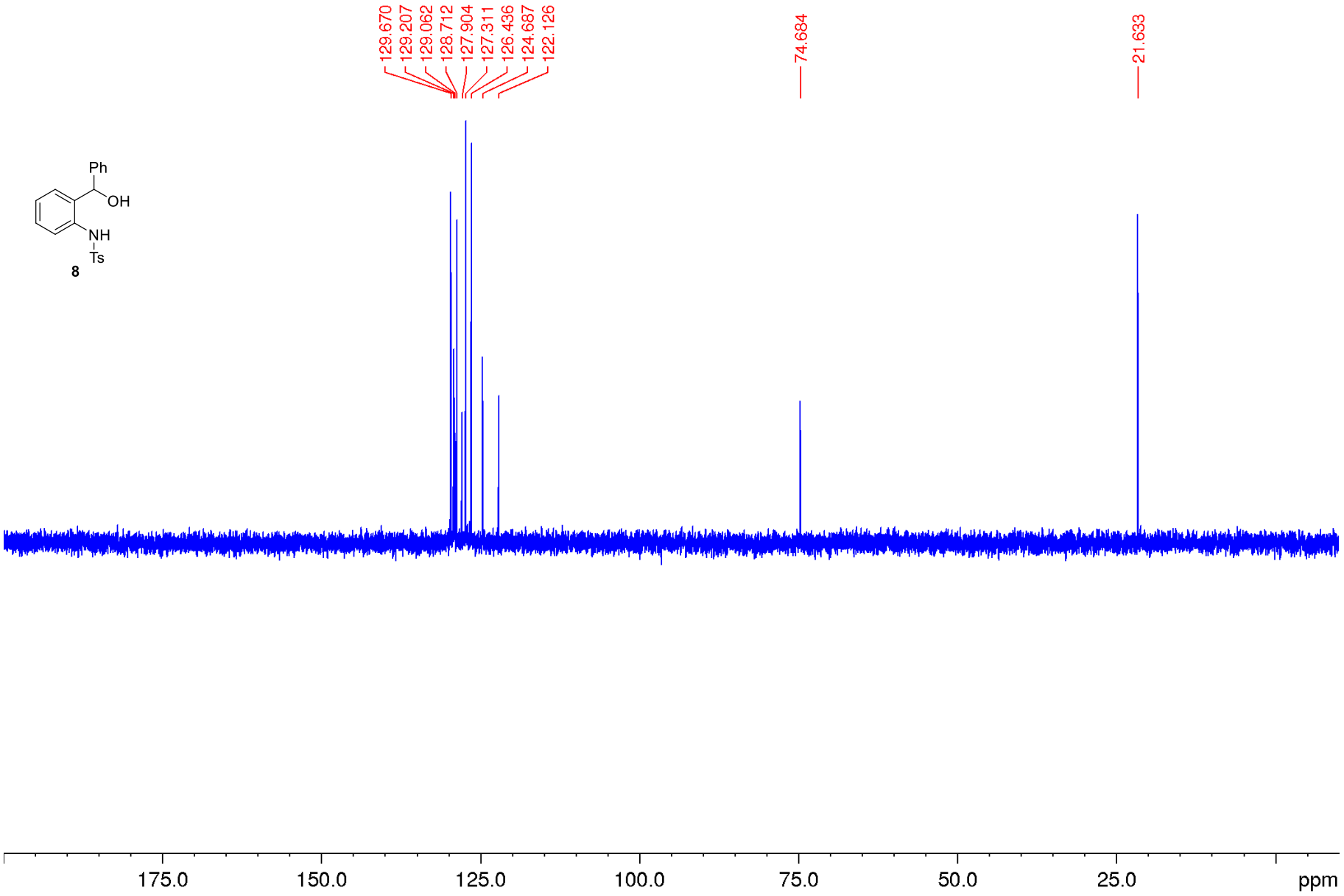
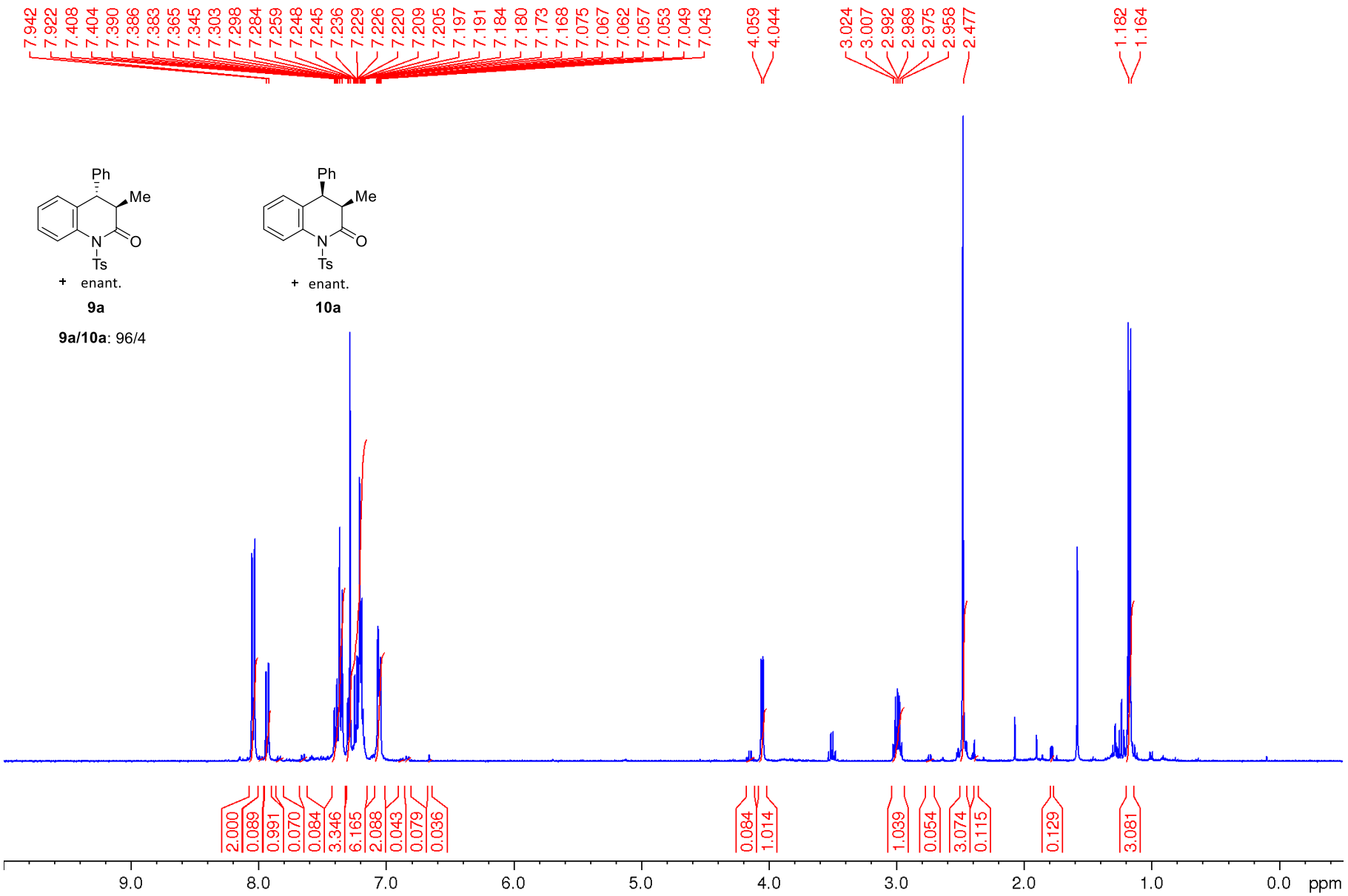
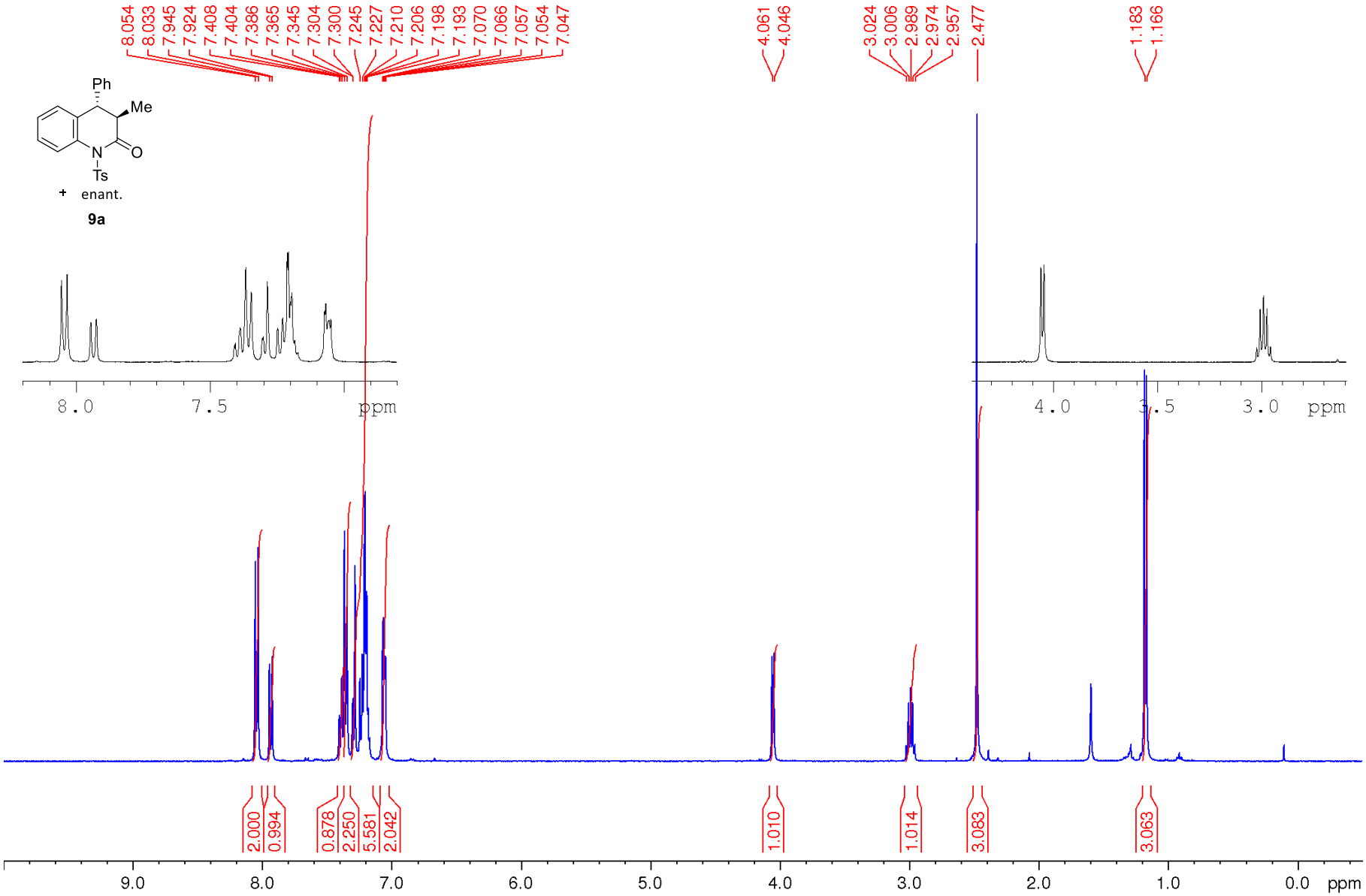
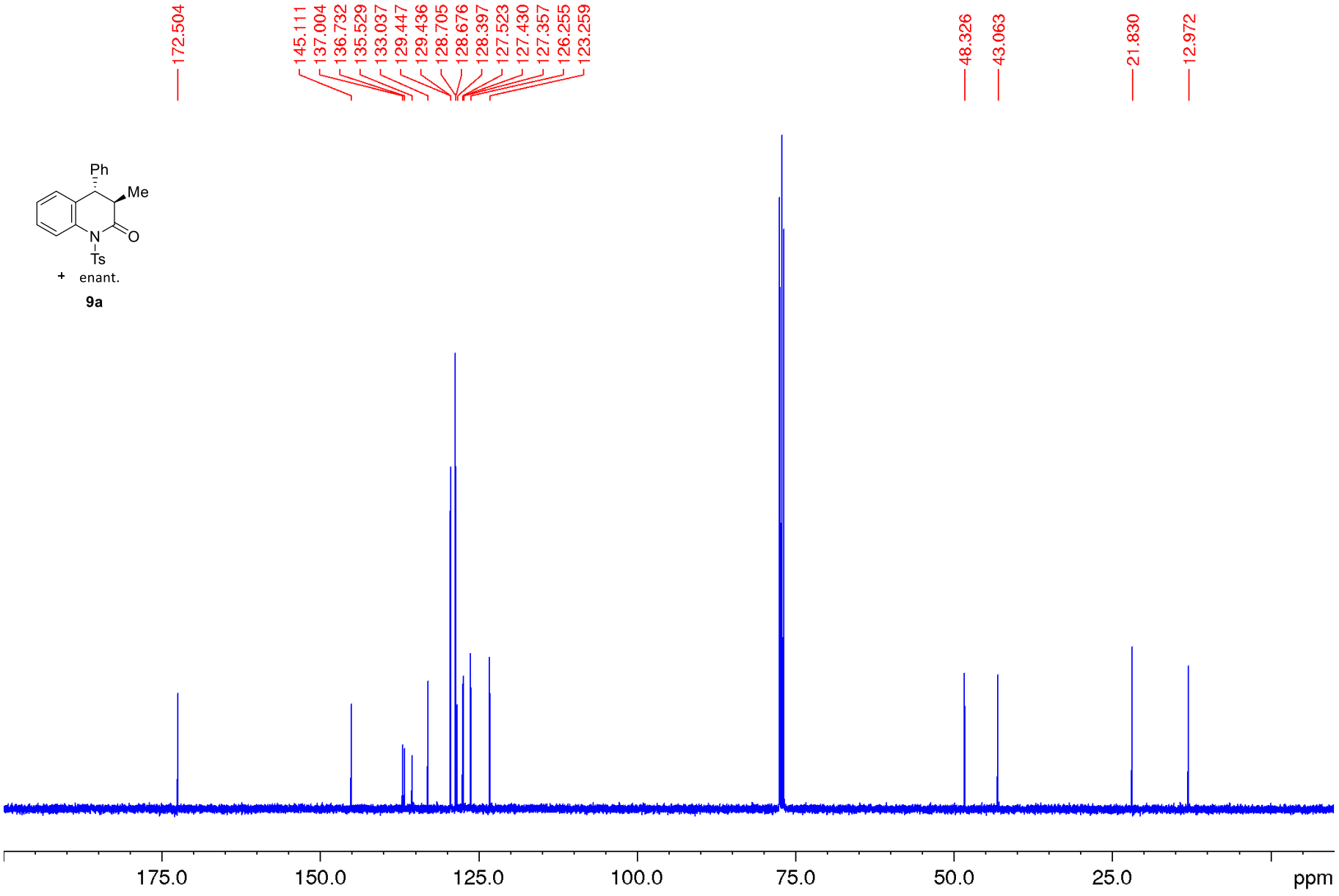
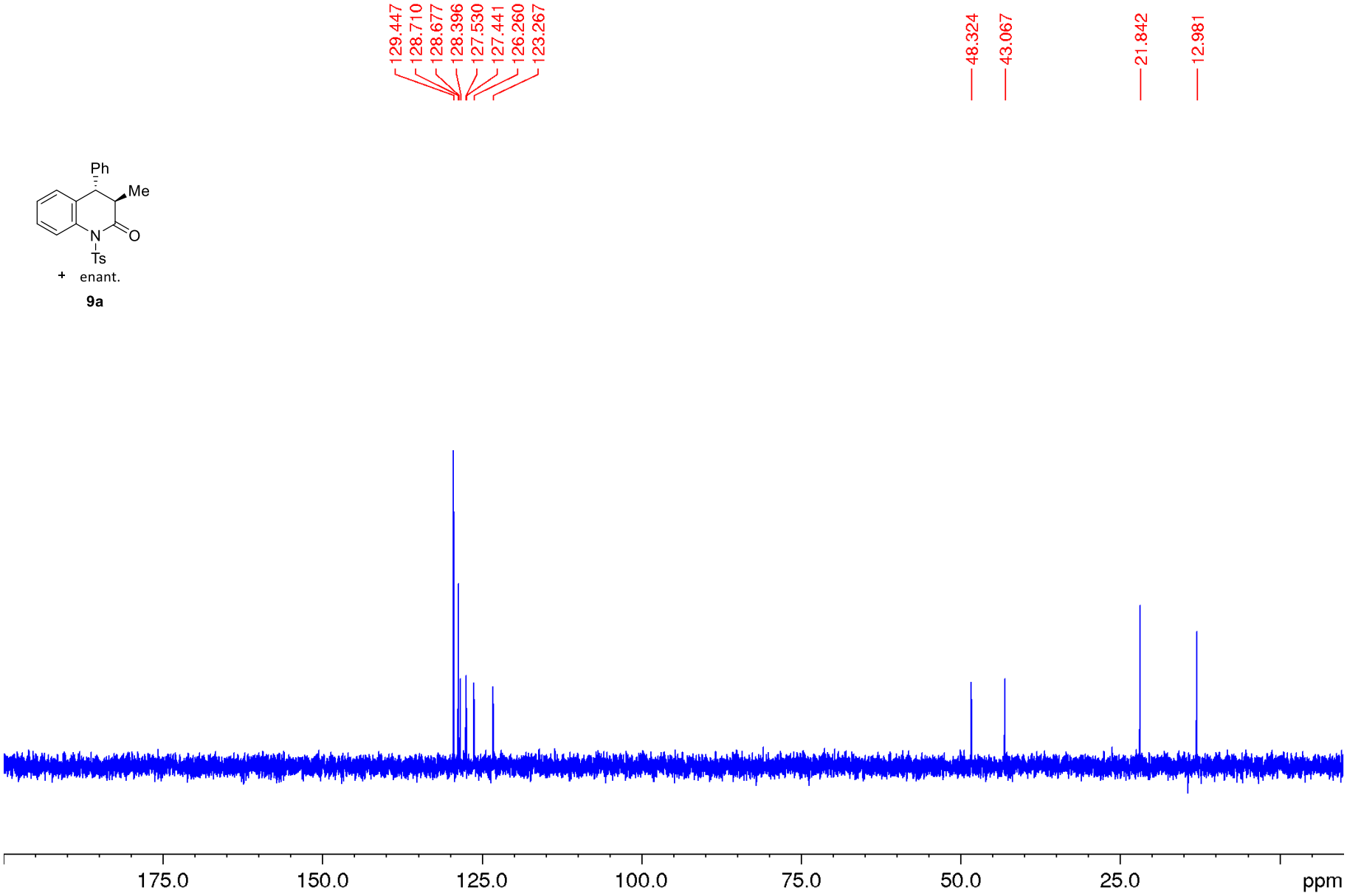
141.125
136.710
135.969
133.205
129.691
129.194
129.152
128.786
128.016
127.342
126.461
124.709
122.206
74.834
21.653
Ph
OH
NH
Ts
8
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

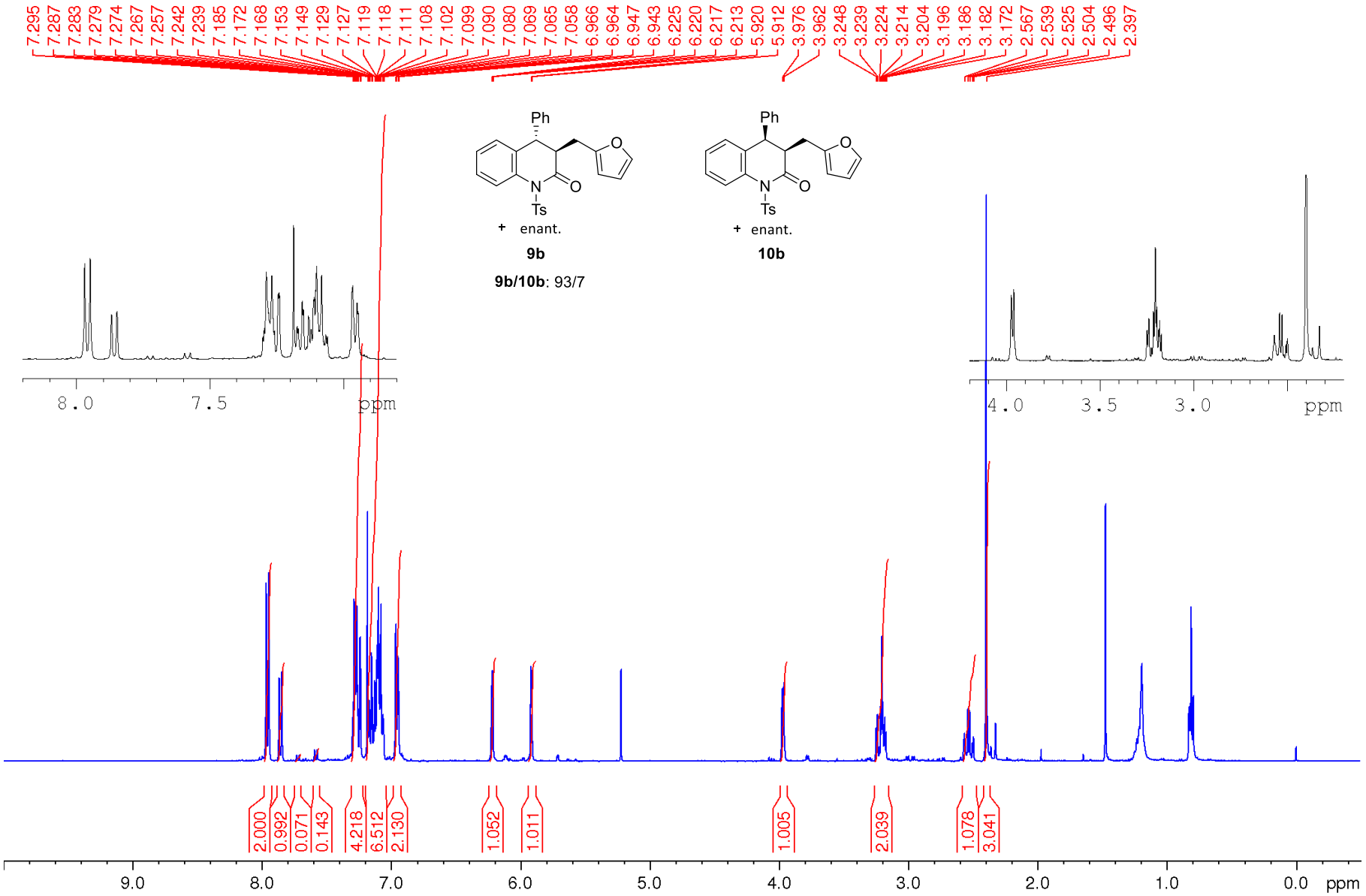

129.670
129.207
129.062
128.712
127.904
127.311
126.436
124.687
122.126
74.684
21.633
Ph
OH
NH
Ts
8
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

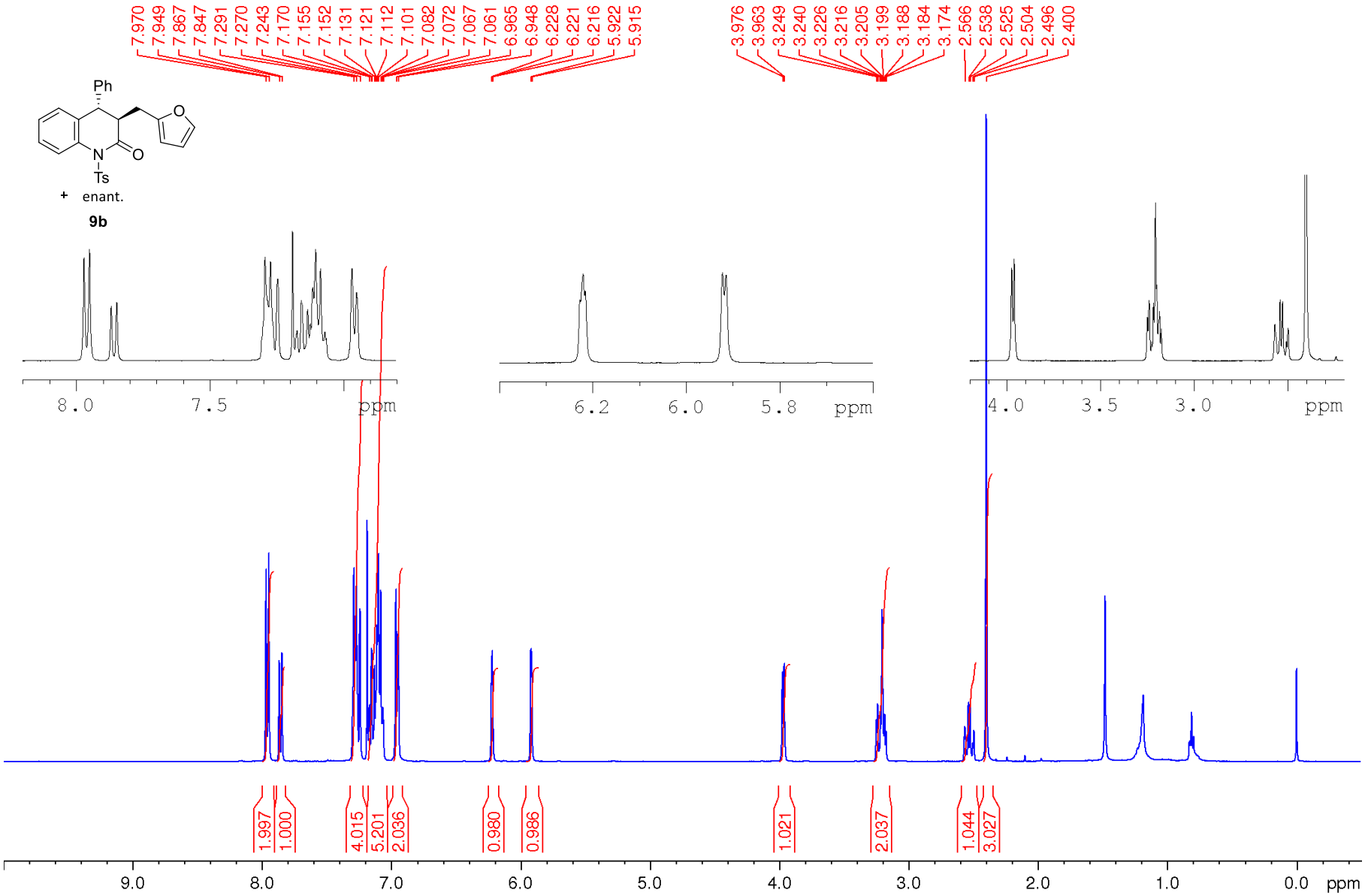

7.942
7.922
7.408
7.404
7.390
7.386
7.383
7.365
7.345
7.303
7.298
7.284
7.259
7.248
7.245
7.236
7.229
7.226
7.220
7.209
7.205
7.197
7.191
7.184
7.180
7.173
7.168
7.075
7.067
7.062
7.057
7.053
7.049
7.043
4.059
4.044
3.024
3.007
2.992
2.989
2.975
2.958
2.477
1.182
1.164
Ph
Me
N
O
Ts
+ enant.
9a
Ph
Me
N
O
Ts
+ enant.
10a
9a/10a: 96/4
2.000
0.089
0.991
0.070
0.084
3.346
6.165
2.088
0.043
0.079
0.036
0.084
1.014
1.039
0.054
3.074
0.115
0.129
3.081
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

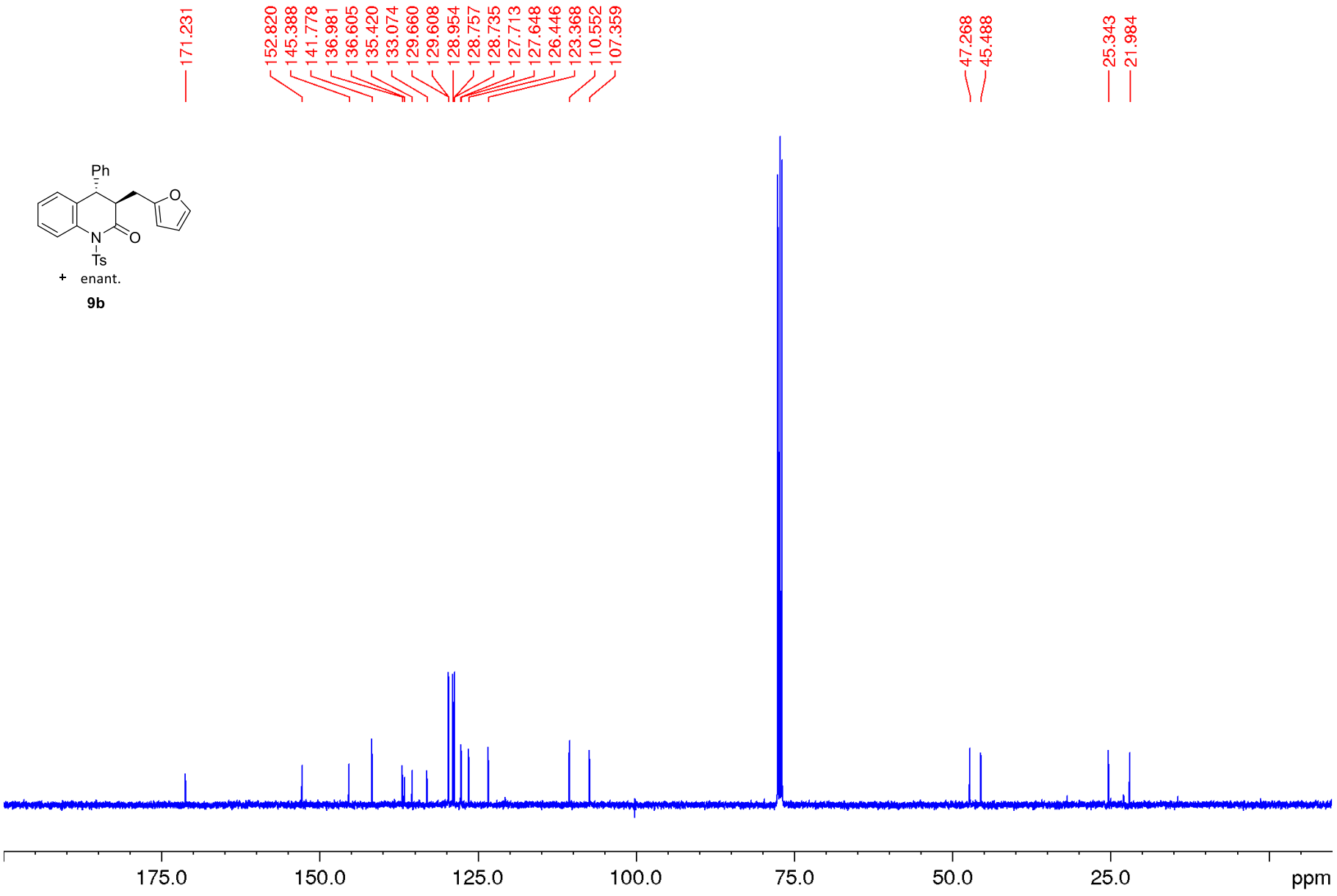

8.054
8.033
7.945
7.924
7.408
7.404
7.386
7.365
7.345
7.304
7.300
7.245
7.227
7.210
7.206
7.198
7.193
7.070
7.066
7.057
7.054
7.047
4.061
4.046
3.024
3.006
2.989
2.974
2.957
2.477
1.183
1.166
Ph
Me
N
O
Ts
+ enant.
9a
8.0
7.5
ppm
4.0
3.5
3.0
ppm
2.000
0.994
0.878
2.250
5.581
2.042
1.010
1.014
3.083
3.063
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

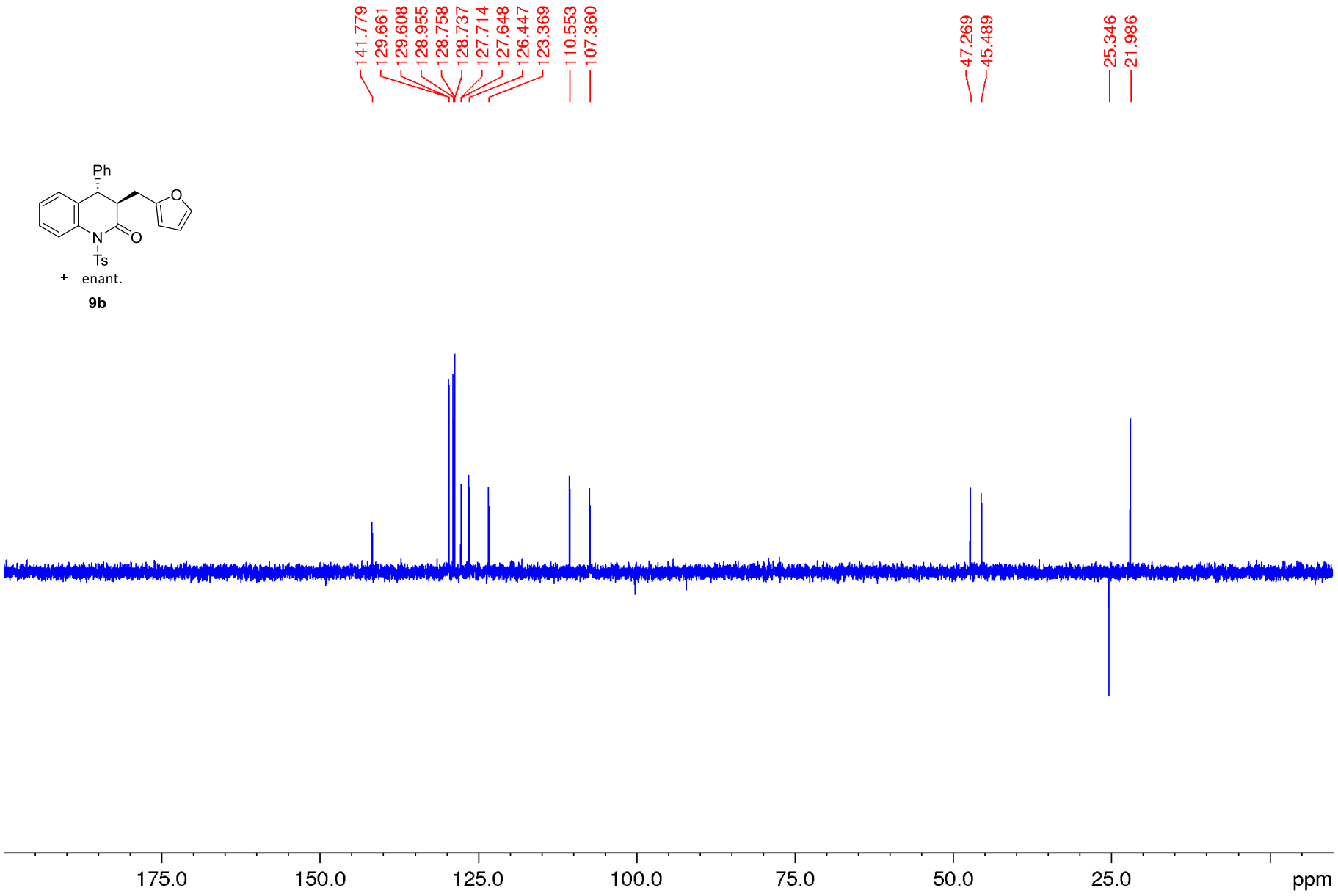

172.504
145.111
137.004
136.732
135.529
133.037
129.447
129.436
128.705
128.676
128.397
127.523
127.430
127.357
126.255
123.259
48.326
43.063
21.830
12.972
Ph
Me
N
O
Ts
+ enant.
9a
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

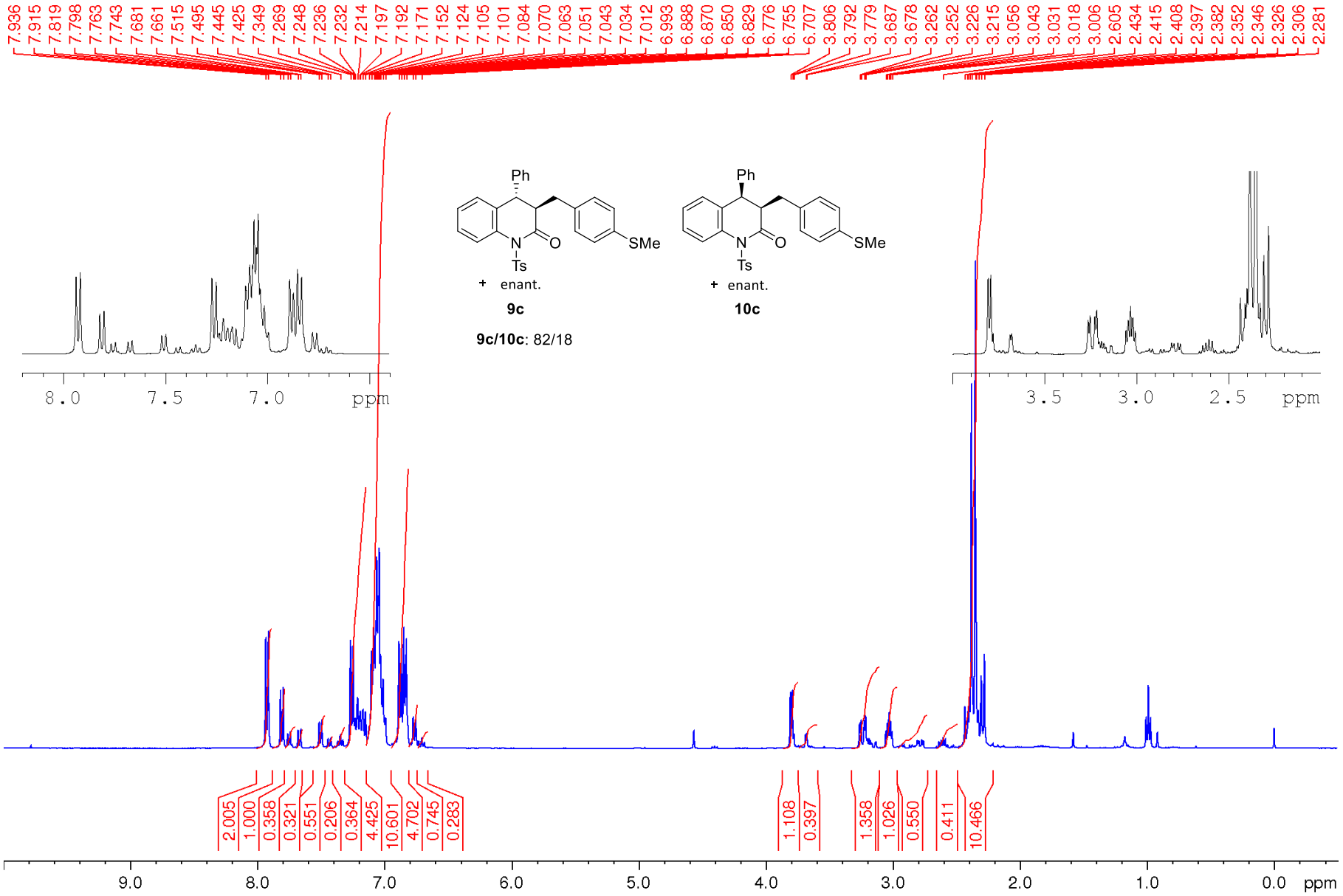

129.447
128.710
128.677
128.396
127.530
127.441
126.260
123.267
48.324
43.067
21.842
12.981
Ph
Me
N
O
Ts
+ enant.
9a
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

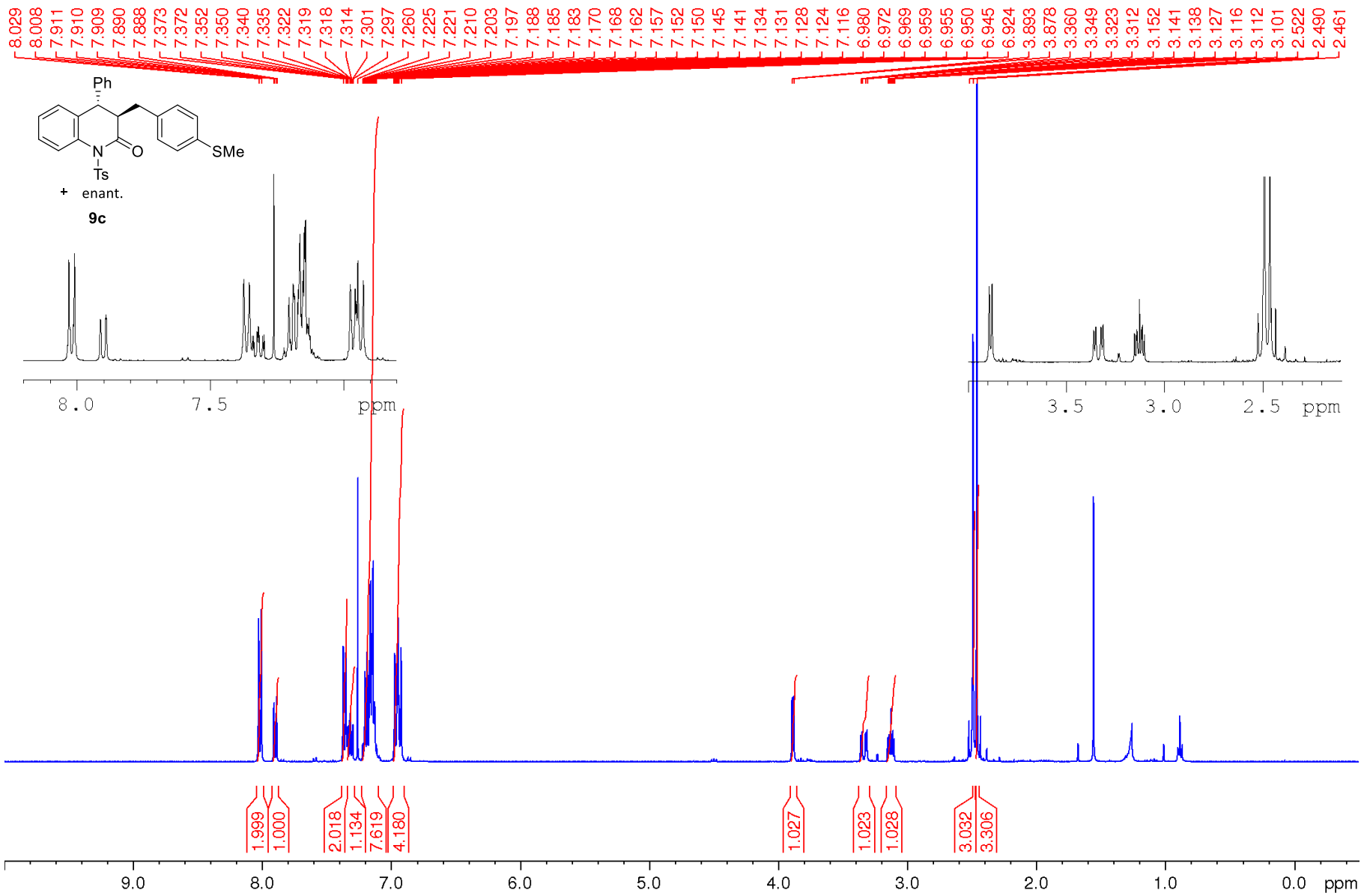

7.295
7.287
7.283
7.279
7.274
7.267
7.257
7.242
7.239
7.185
7.172
7.168
7.153
7.149
7.129
7.127
7.119
7.118
7.111
7.108
7.102
7.099
7.090
7.080
7.069
7.065
7.058
6.966
6.964
6.947
6.943
6.225
6.220
6.217
6.213
5.920
5.912
3.976
3.962
3.248
3.239
3.224
3.214
3.204
3.196
3.186
3.182
3.172
2.567
2.539
2.525
2.504
2.496
2.397
Ph
O
N
O
Ts
+ enant.
9b
9b/10b: 93/7
Ph
O
N
O
Ts
+ enant.
10b
8.0
7.5
ppm
4.0
3.5
3.0
ppm
2.000
0.992
0.071
0.143
4.218
6.512
2.130
1.052
1.011
1.005
2.039
1.078
3.041
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


7.970
7.949
7.867
7.847
7.291
7.270
7.243
7.170
7.155
7.152
7.131
7.121
7.112
7.101
7.082
7.072
7.067
7.061
6.965
6.948
6.228
6.221
6.216
5.922
5.915
3.976
3.963
3.249
3.240
3.226
3.216
3.205
3.199
3.188
3.184
3.174
2.566
2.538
2.525
2.504
2.496
2.400
Ph
O
N
O
Ts
+ enant.
9b
8.0
7.5
ppm
6.2
6.0
5.8
ppm
4.0
3.5
3.0
ppm
1.997
1.000
4.015
5.201
2.036
0.980
0.986
1.021
2.037
1.044
3.027
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


171.231
152.820
145.388
141.778
136.981
136.605
135.420
133.074
129.660
129.608
128.954
128.757
128.735
127.713
127.648
126.446
123.368
110.552
107.359
47.268
45.488
25.343
21.984
Ph
O
N
O
Ts
+ enant.
9b
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


141.779
129.661
129.608
128.955
128.758
128.737
127.714
127.648
126.447
123.369
110.553
107.360
47.269
45.489
25.346
21.986
Ph
O
N
O
Ts
+ enant.
9b
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


7.936 7.915 7.819 7.798 7.763 7.743 7.681 7.661 7.515 7.495 7.445 7.425 7.349 7.269 7.248 7.236 7.232 7.214 7.197 7.192 7.171 7.152 7.124 7.105 7.101 7.084 7.070 7.063 7.051 7.043 7.034 7.012 6.993 6.888 6.870 6.850 6.829 6.776 6.755 6.707 3.806 3.792 3.779 3.687 3.678 3.262 3.252 3.226 3.215 3.056 3.043 3.031 3.018 3.006 2.605 2.434 2.415 2.408 2.397 2.382 2.352 2.346 2.326 2.306 2.281
Ph
N
O
Ts
SMe
+ enant.
9c
9c/10c: 82/18
Ph
N
O
Ts
SMe
+ enant.
10c
8.0 7.5 7.0 ppm
3.5 3.0 2.5 ppm
2.005 1.000 0.358 0.321 0.551 0.206 0.364 4.425 10.601 4.702 0.745 0.283
1.108 0.397 1.358 1.026 0.550 0.411 10.466
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 ppm


8.029
8.008
7.911
7.910
7.909
7.890
7.888
7.373
7.372
7.352
7.350
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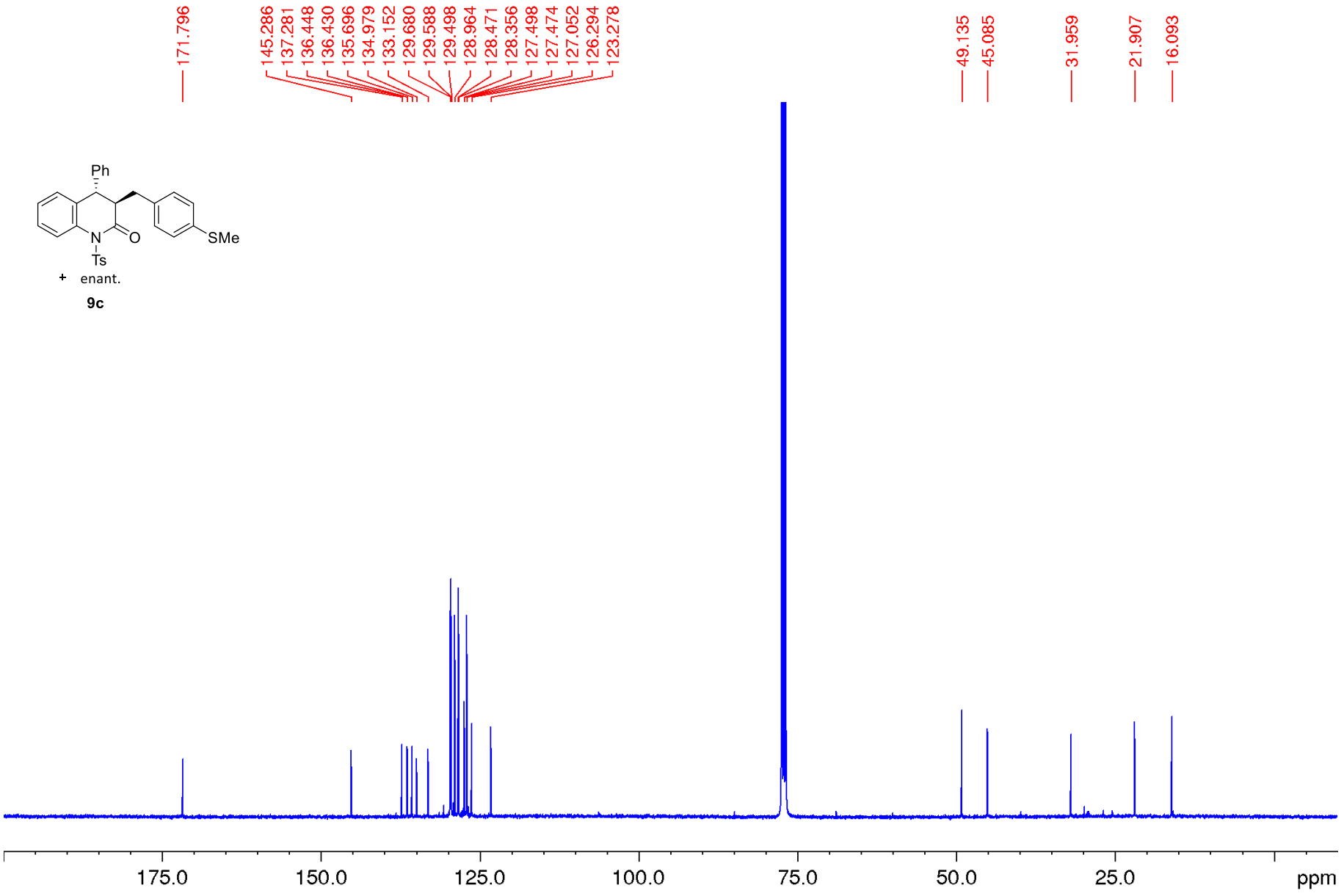
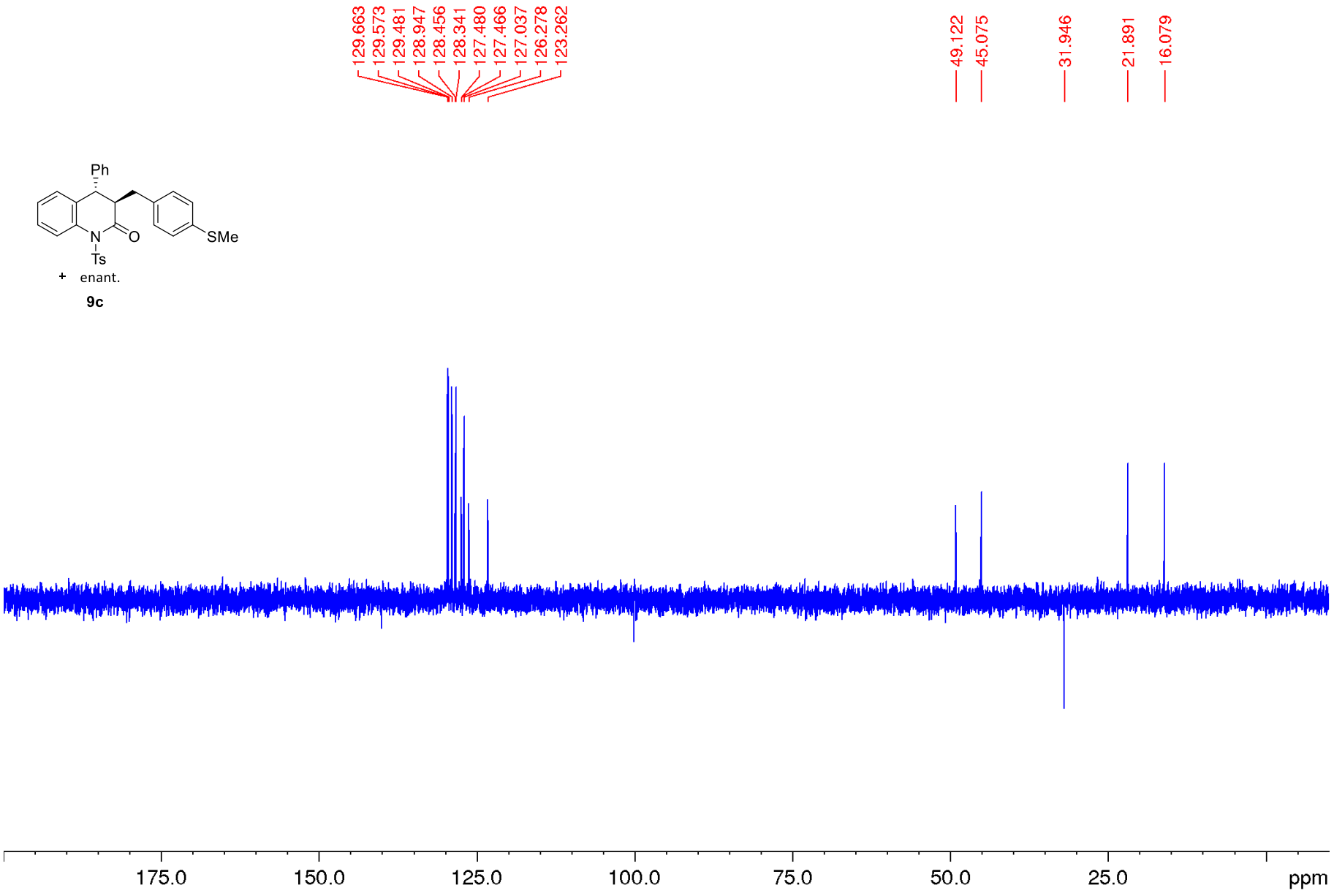
7.335
7.322
7.319
7.318
7.314
7.301
7.297
7.260
7.225
7.221
7.210
7.203
7.197
7.188
7.185
7.183
7.170
7.168
7.162
7.157
7.152
7.150
7.145
7.141
7.134
7.131
7.128
7.124
7.116
6.980
6.972
6.969
6.959
6.955
6.950
6.945
6.924
3.893
3.878
3.360
3.349
3.323
3.312
3.152
3.141
3.138
3.127
3.116
3.112
3.101
2.522
2.490
2.461
Ph
N
O
SMe
Ts
+ enant.
9c
8.0
7.5
ppm
3.5
3.0
2.5
ppm
1.999
1.000
2.018
1.134
7.619
4.180
1.027
1.023
1.028
3.032
3.306
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


171.796
145.286
137.281
136.448
136.430
135.696
134.979
133.152
129.680
129.588
129.498
128.964
128.471
128.356
127.498
127.474
127.052
126.294
123.278
49.135
45.085
31.959
21.907
16.093
Ph
N
O
Ts
SMe
+ enant.
9c
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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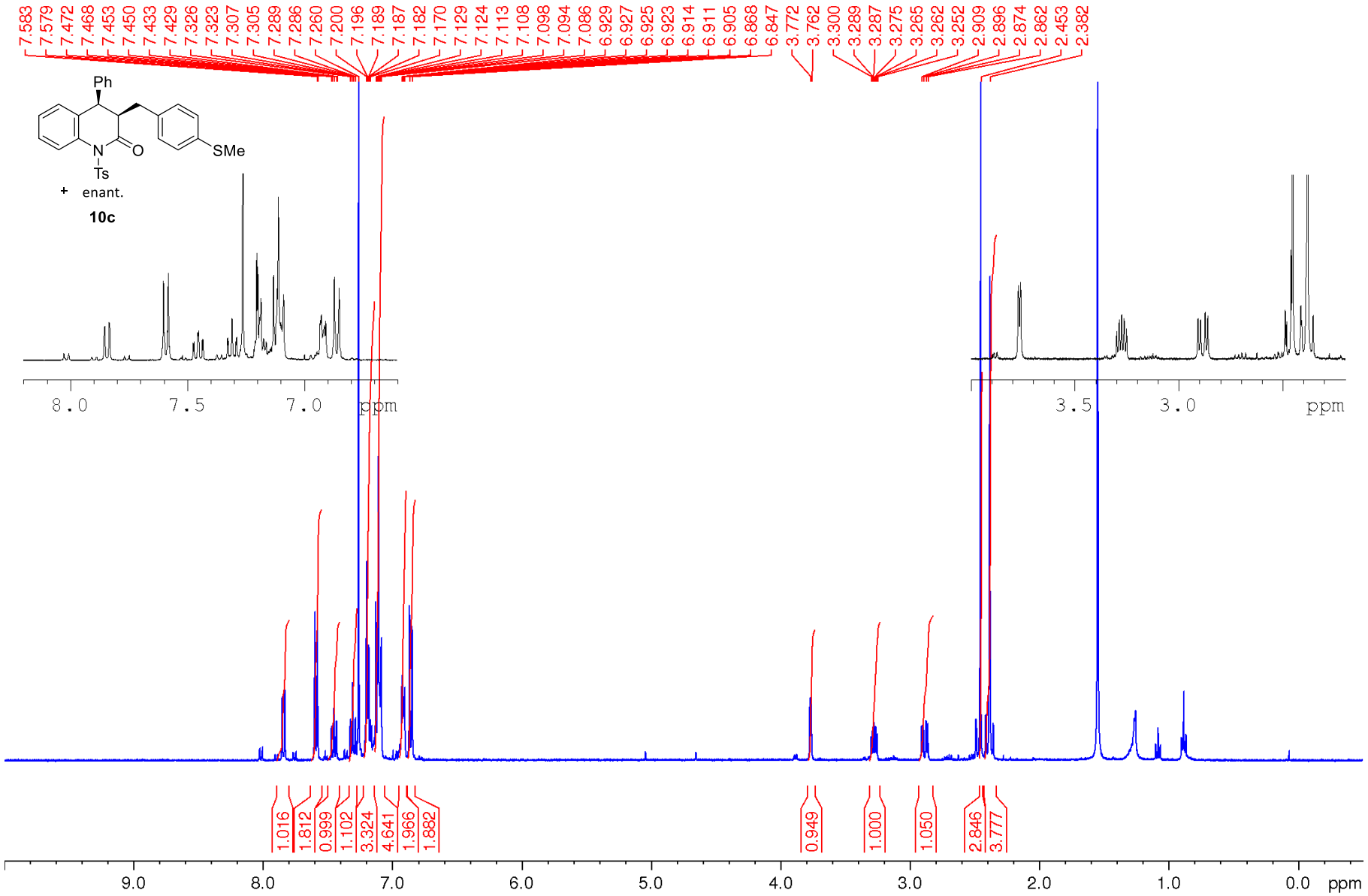
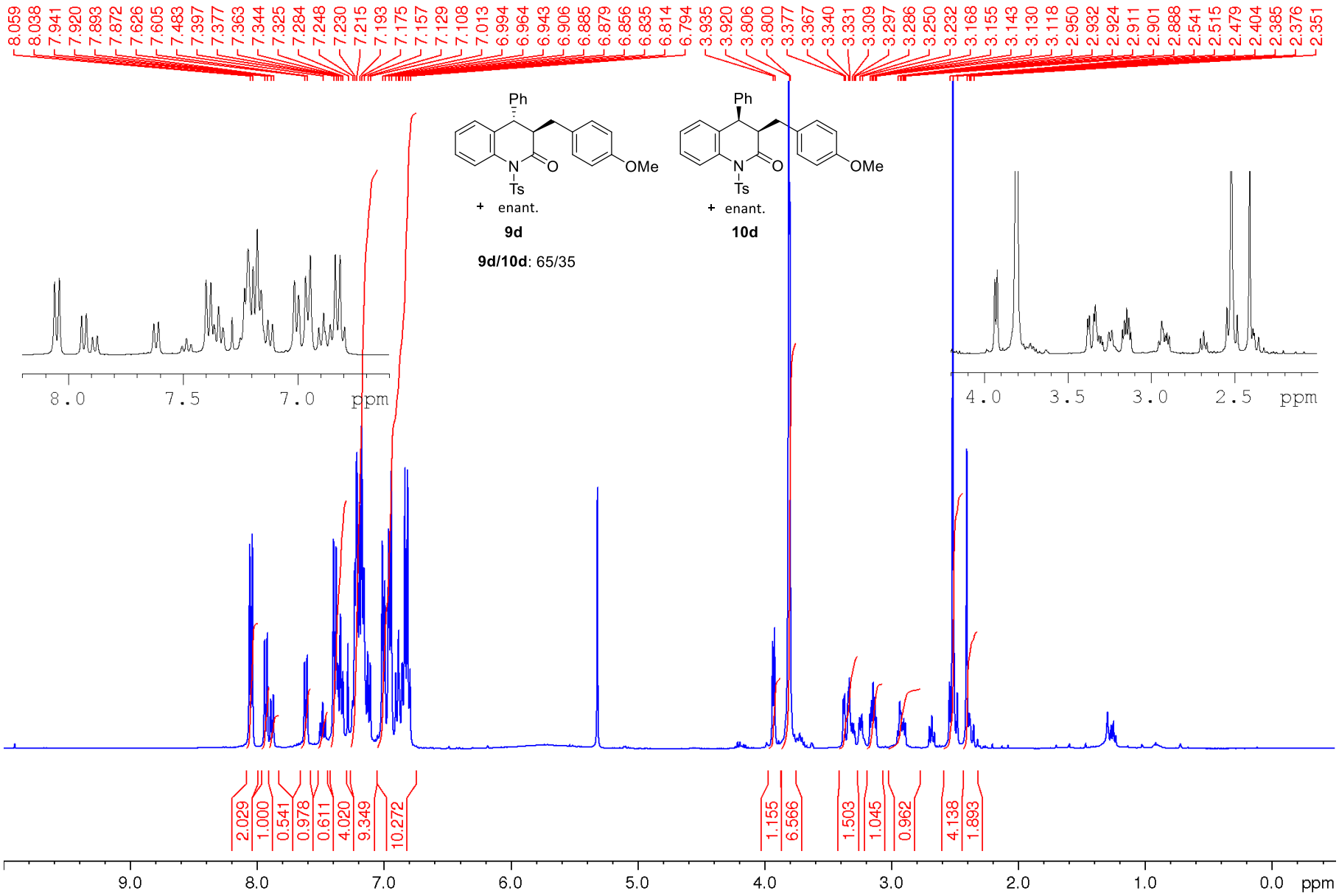
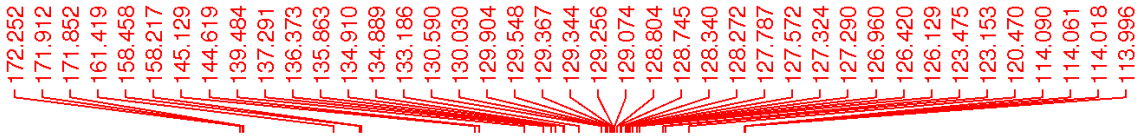
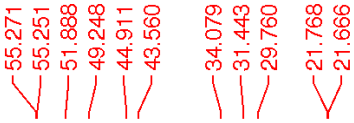
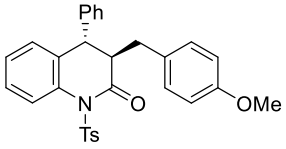
129.573
129.481
128.947
128.456
128.341
127.480
127.466
127.037
126.278
123.262
49.122
45.075
31.946
21.891
16.079
Ph
N
O
Ts
SMe
+ enant.
9c
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


7.583
7.579
7.472
7.468
7.453
7.450
7.433
7.429
7.326
7.323
7.307
7.305
7.289
7.286
7.260
7.200
7.196
7.189
7.187
7.182
7.170
7.129
7.124
7.113
7.108
7.098
7.094
7.086
6.929
6.927
6.925
6.923
6.914
6.911
6.905
6.868
6.847
3.772
3.762
3.300
3.289
3.287
3.275
3.265
3.262
3.252
2.909
2.896
2.874
2.862
2.453
2.382
Ph
N
O
SMe
Ts
+ enant.
10c
8.0
7.5
7.0
ppm
3.5
3.0
ppm
1.016
1.812
0.999
1.102
3.324
4.641
1.966
1.882
0.949
1.000
1.050
2.846
3.777
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


8.059 8.038 7.941 7.920 7.893 7.872 7.626 7.605 7.483 7.397 7.377 7.363 7.344 7.325 7.284 7.248 7.230 7.215 7.193 7.175 7.157 7.129 7.108 7.013 6.994 6.964 6.943 6.906 6.885 6.879 6.856 6.835 6.814 6.794
3.935 3.920 3.806 3.800 3.377 3.367 3.340 3.331 3.309 3.297 3.286 3.250 3.232 3.168 3.155 3.143 3.130 3.118 2.950 2.932 2.924 2.911 2.901 2.888 2.541 2.515 2.479 2.404 2.385 2.376 2.351
Ph
N
O
Ts
OMe
+ enant.
9d
9d/10d: 65/35
10d
8.0 7.5 7.0 ppm
4.0 3.5 3.0 2.5 ppm
2.029 1.000 0.541 0.978 0.611 4.020 9.349 10.272
1.155 6.566 1.503 1.045 0.962 4.138 1.893
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 ppm

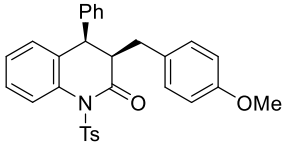






+ enant.

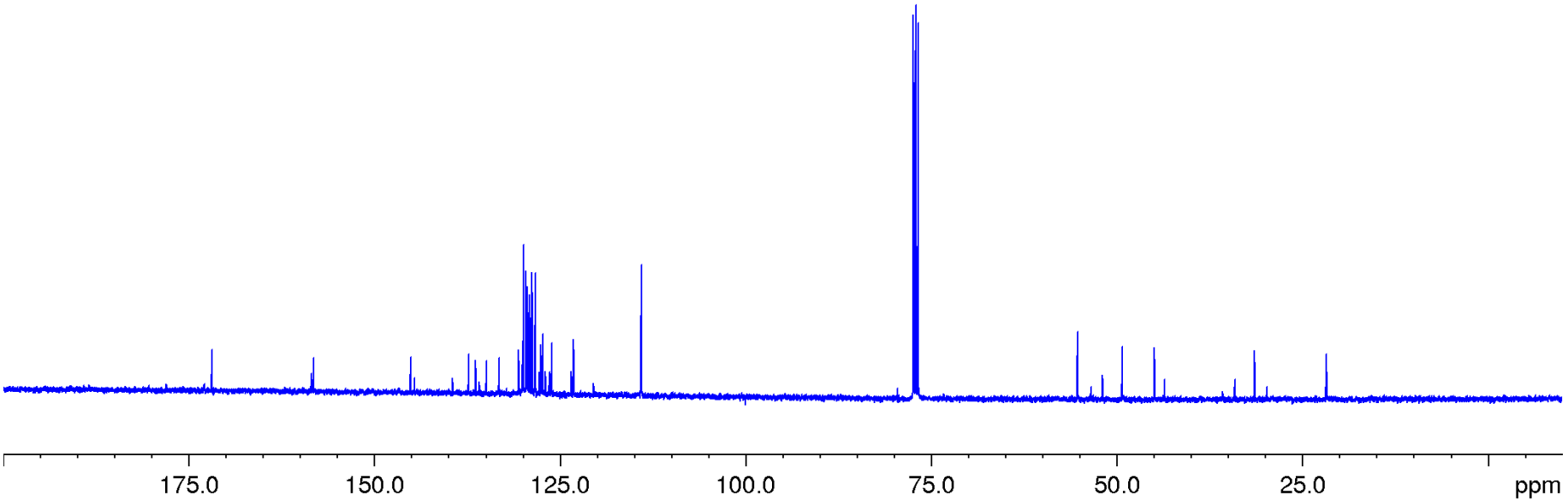
9d

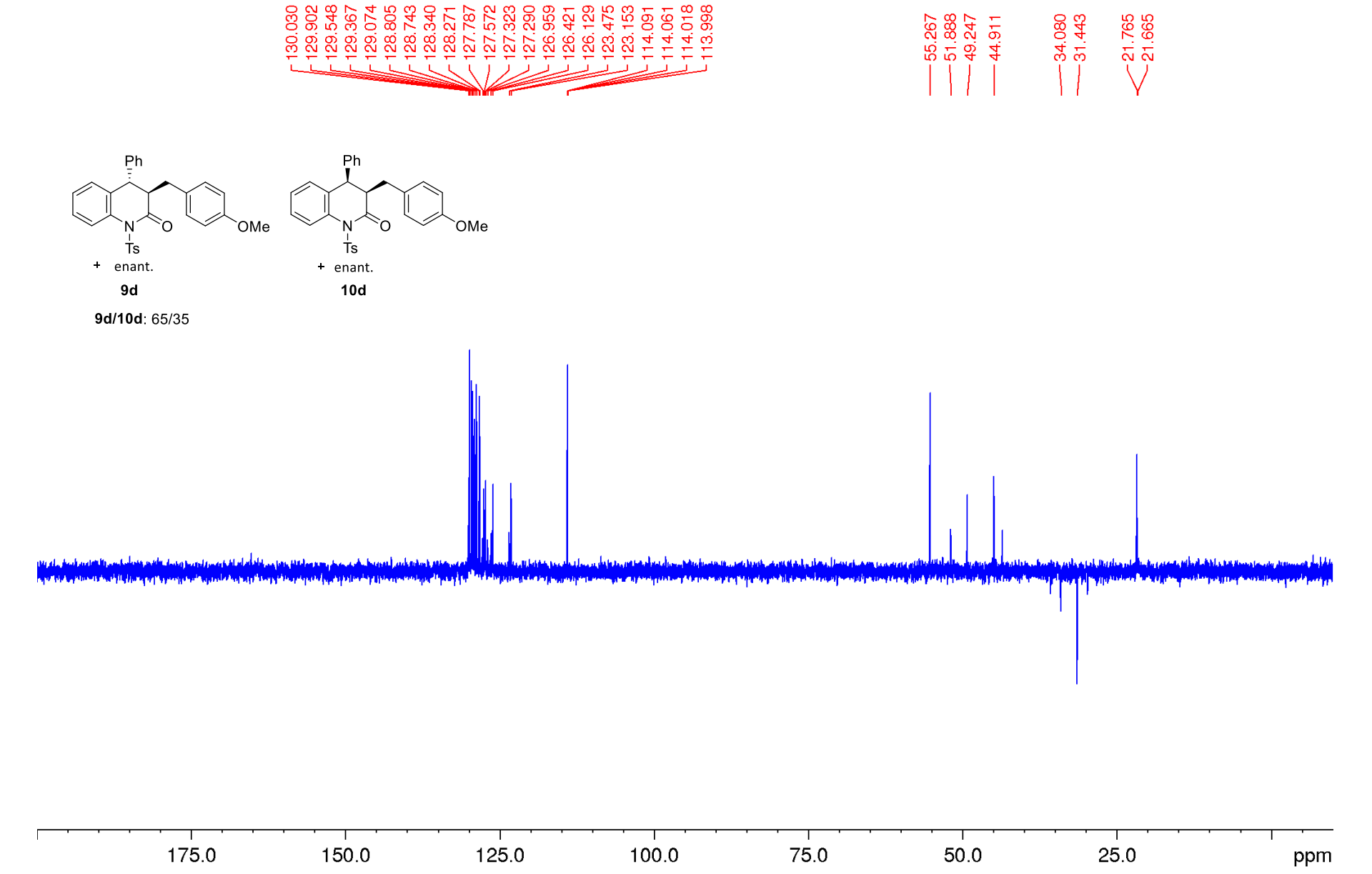


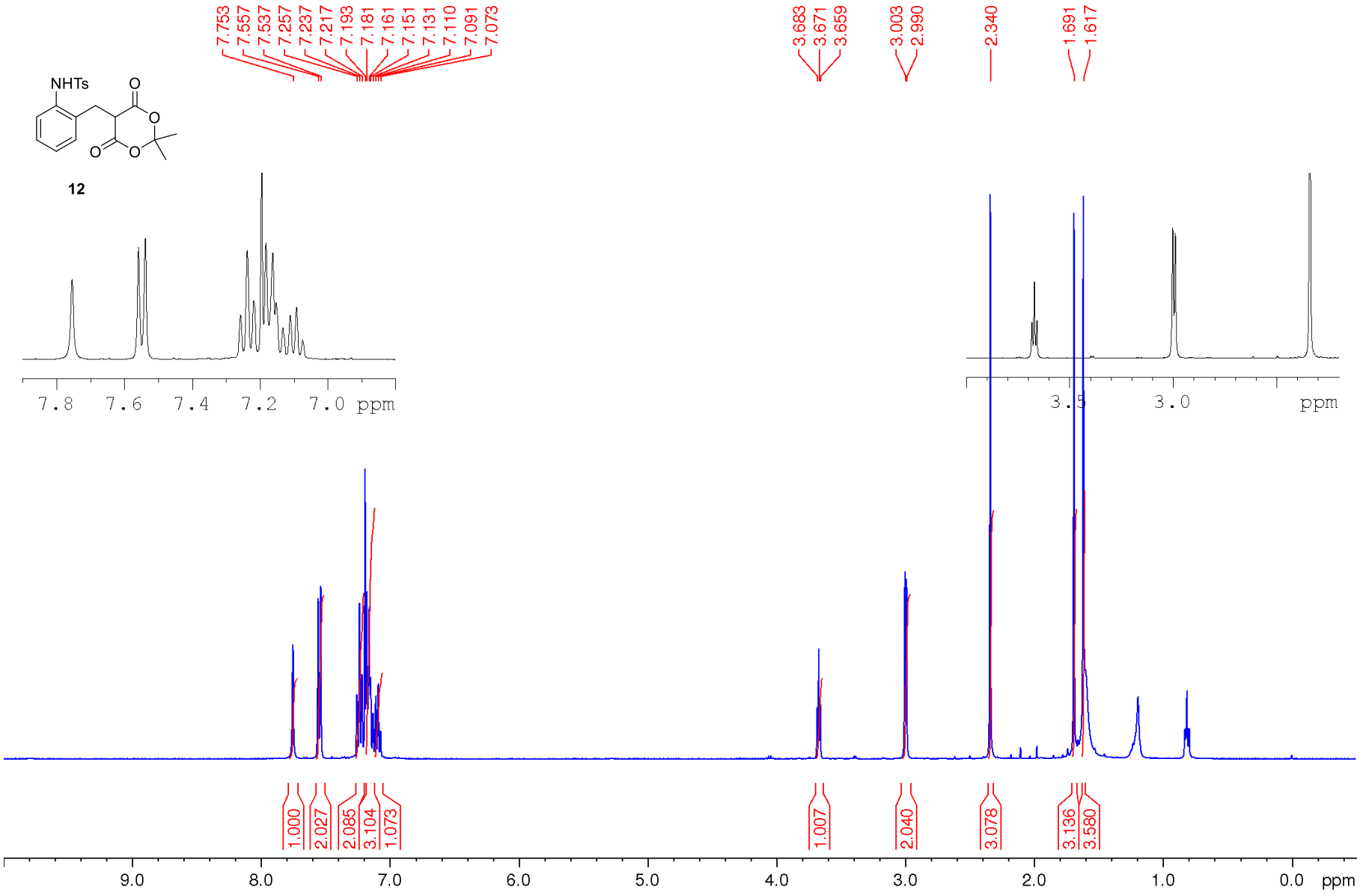
+ enant.

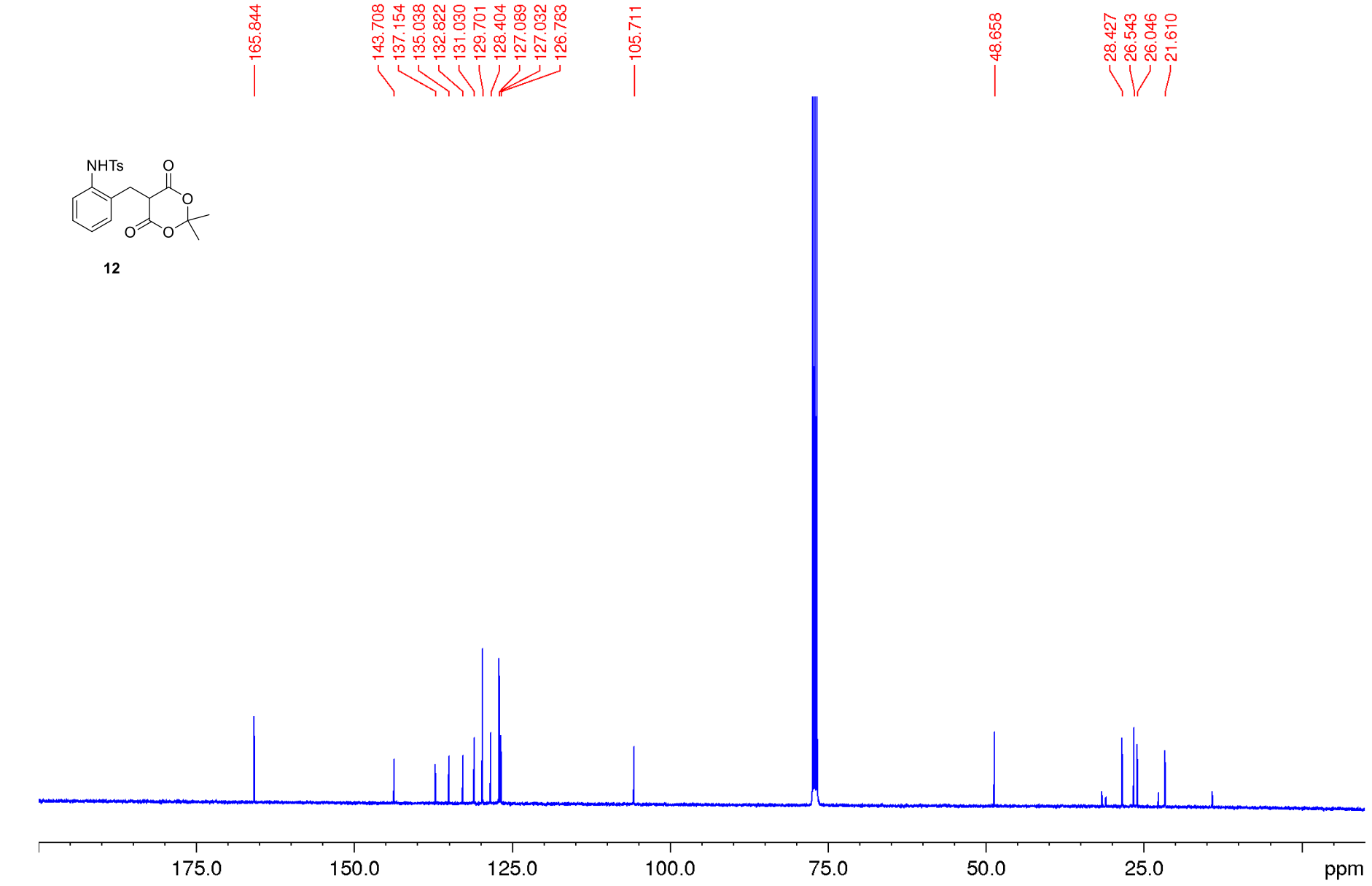
10d

9d/10d: 65/35

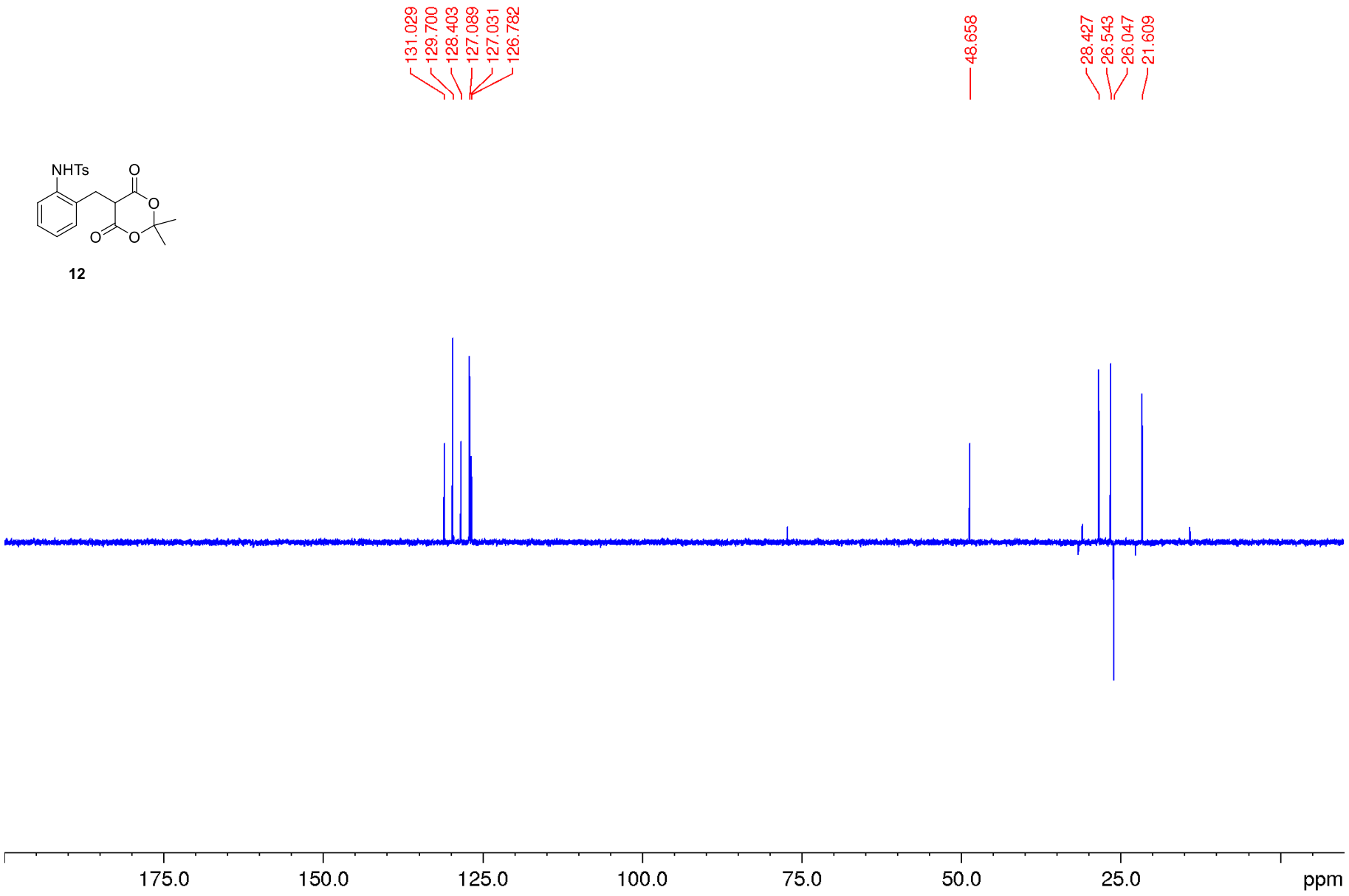



130.030
129.902
129.548
129.367
129.074
128.805
128.743
128.340
128.271
127.787
127.572
127.323
127.290
126.959
126.421
126.129
123.475
123.153
114.091
114.061
114.018
113.998
55.267
51.888
49.247
44.911
34.080
31.443
21.765
21.665
Ph
N
O
Ts
OMe
+ enant.
9d
Ph
N
O
Ts
OMe
+ enant.
10d
9d/10d: 65/35
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

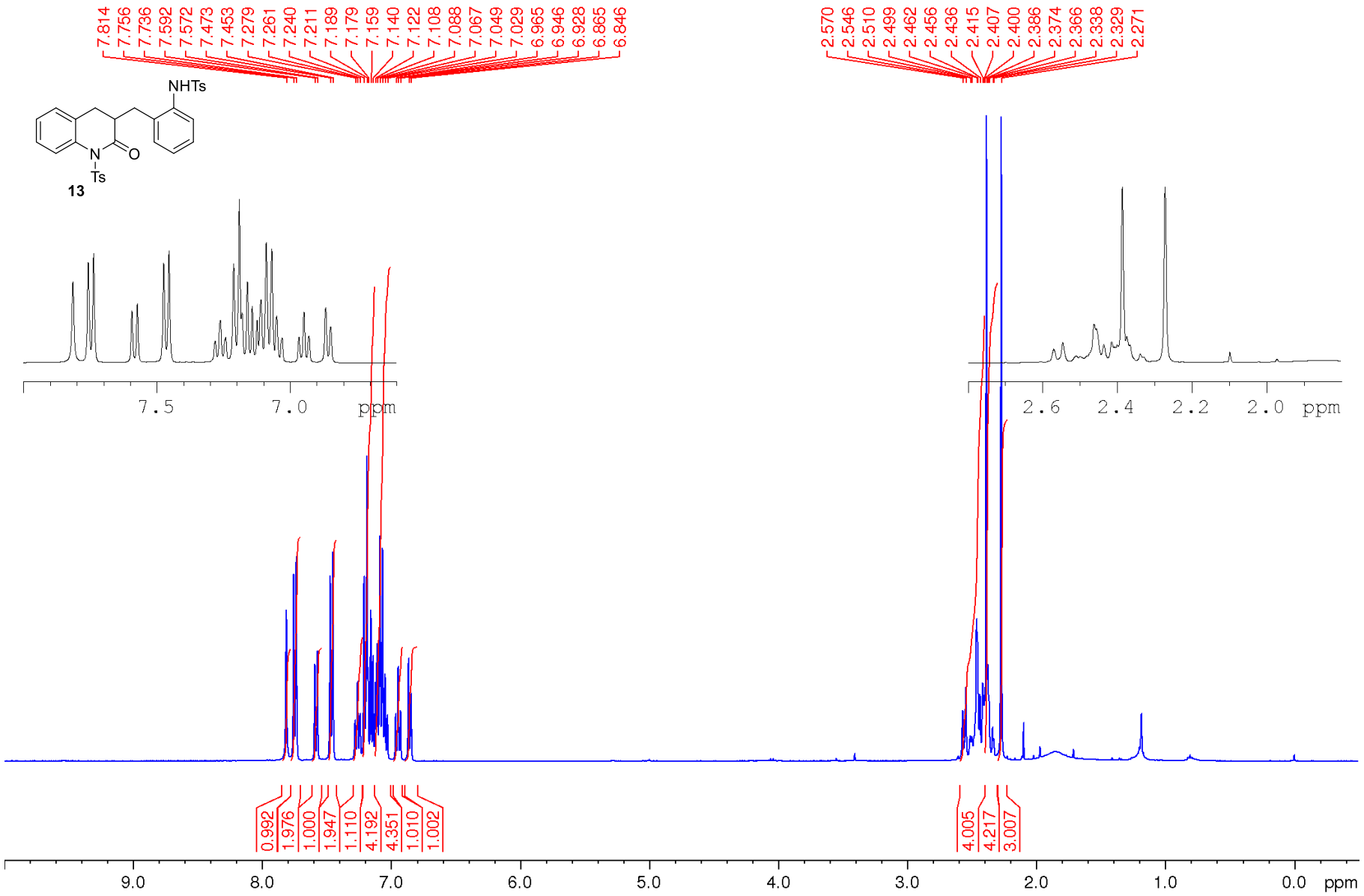

7.753
7.557
7.537
7.257
7.237
7.217
7.193
7.181
7.161
7.151
7.131
7.110
7.091
7.073
3.683
3.671
3.659
3.003
2.990
2.340
1.691
1.617
NHTs
O
O
O
O
12
7.8
7.6
7.4
7.2
7.0 ppm
3.5
3.0
ppm
1.000
2.027
2.085
3.104
1.073
1.007
2.040
3.078
3.136
3.580
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0 ppm


165.844
143.708
137.154
135.038
132.822
131.030
129.701
128.404
127.089
127.032
126.783
105.711
48.658
28.427
26.543
26.046
21.610
NHTs
O
O
O
O
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

12


131.029
129.700
128.403
127.089
127.031
126.782
48.658
28.427
26.543
26.047
21.609
NHTs
O
O
O
O
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

12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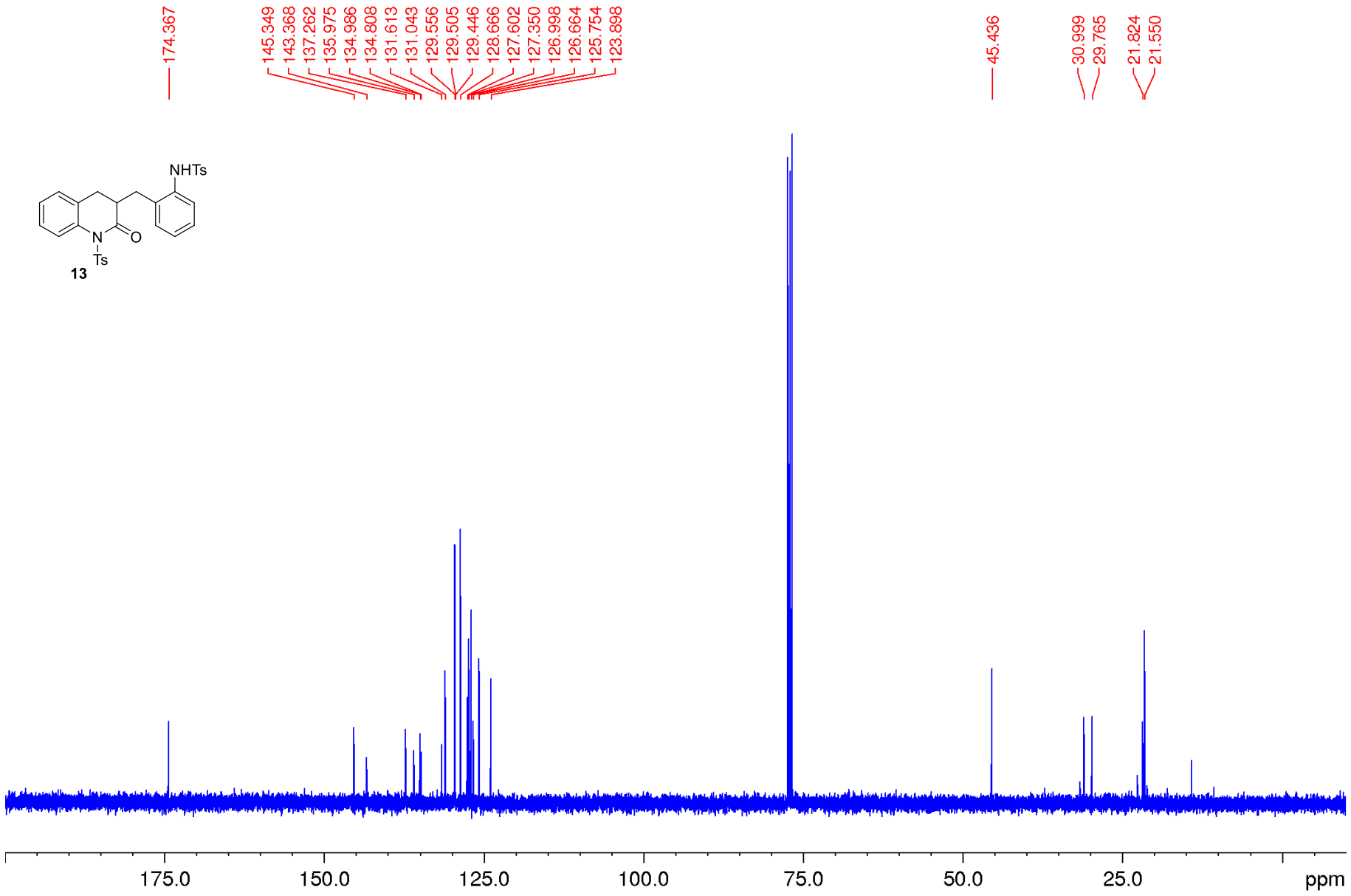
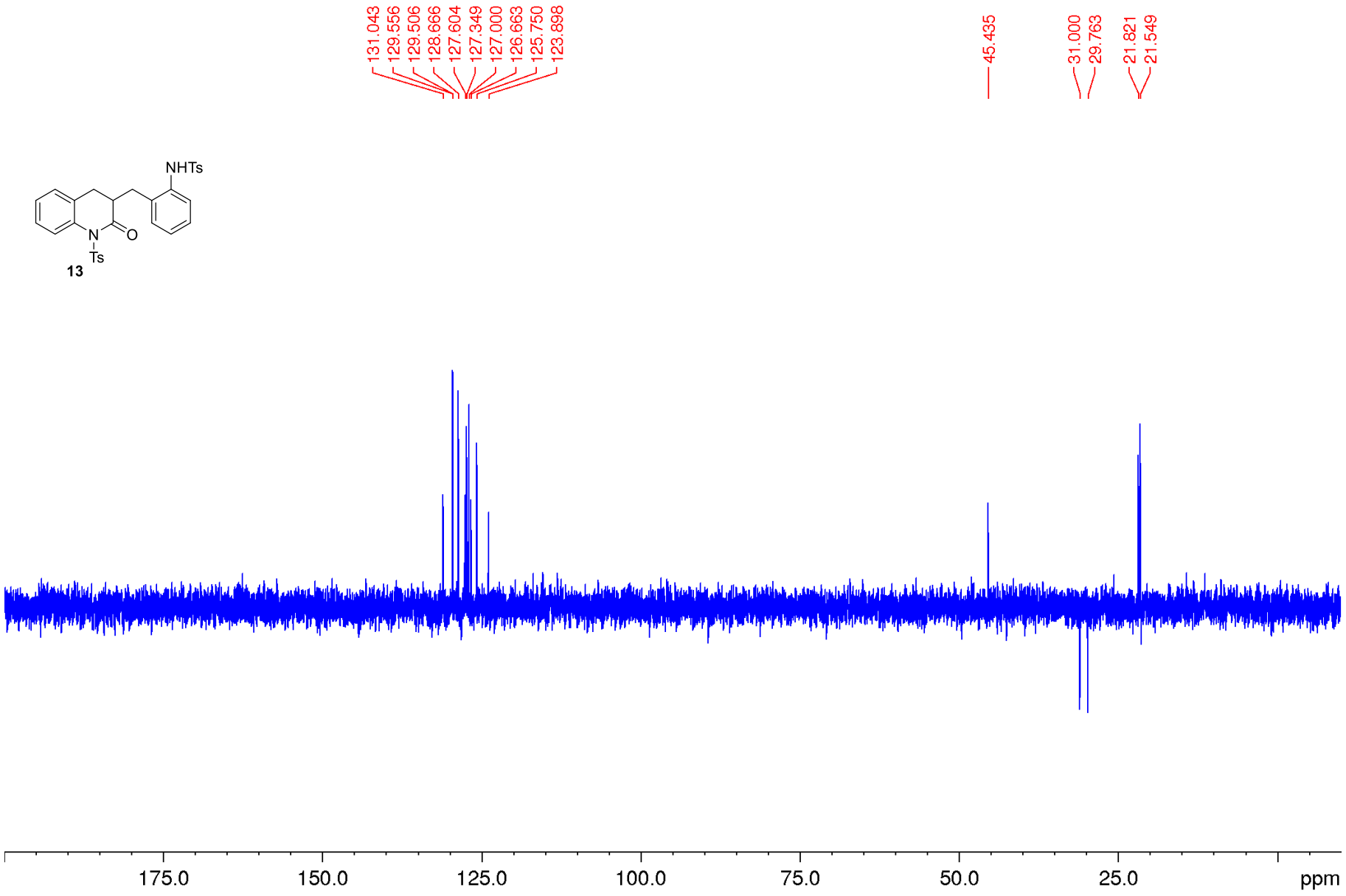
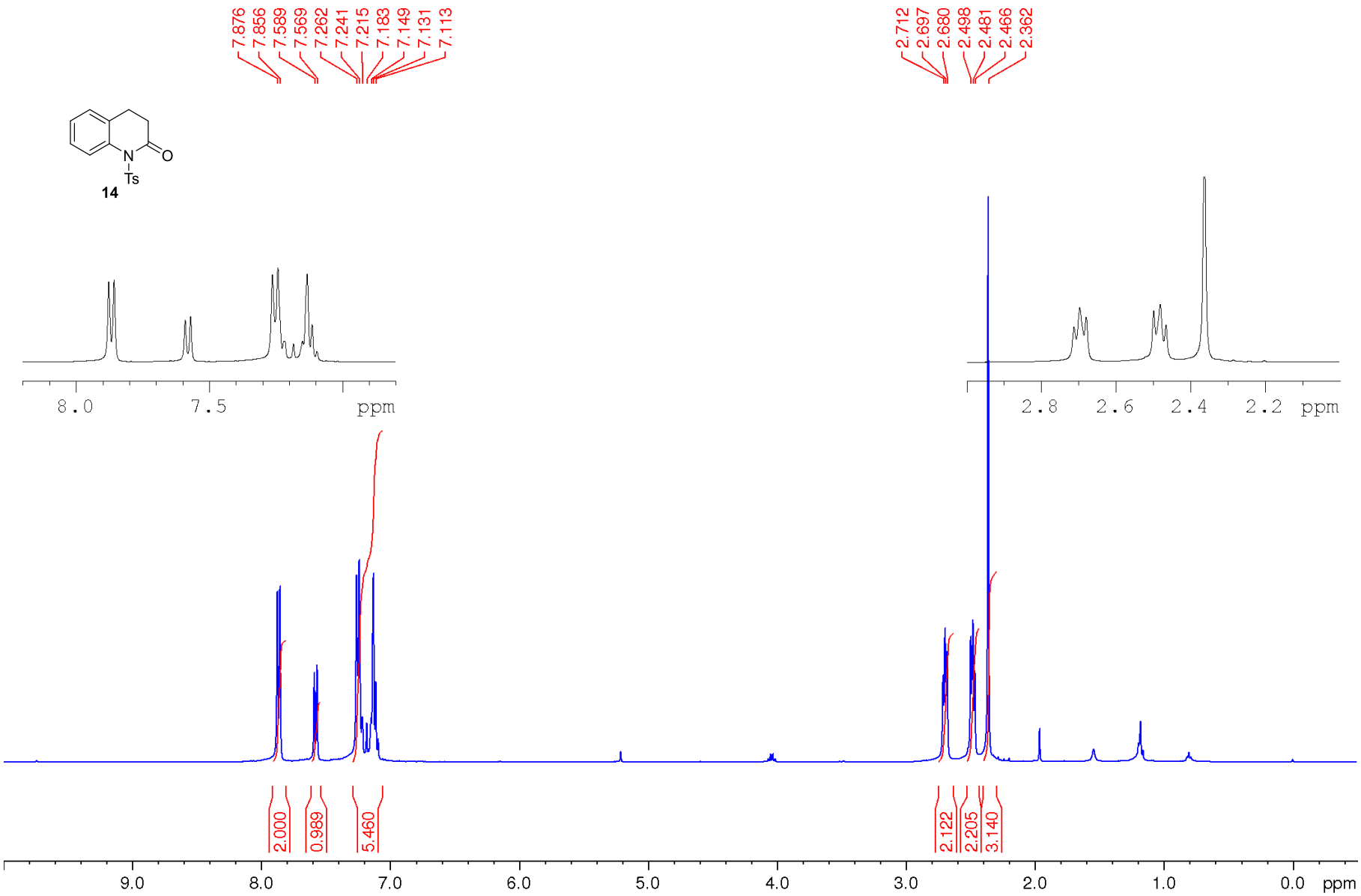
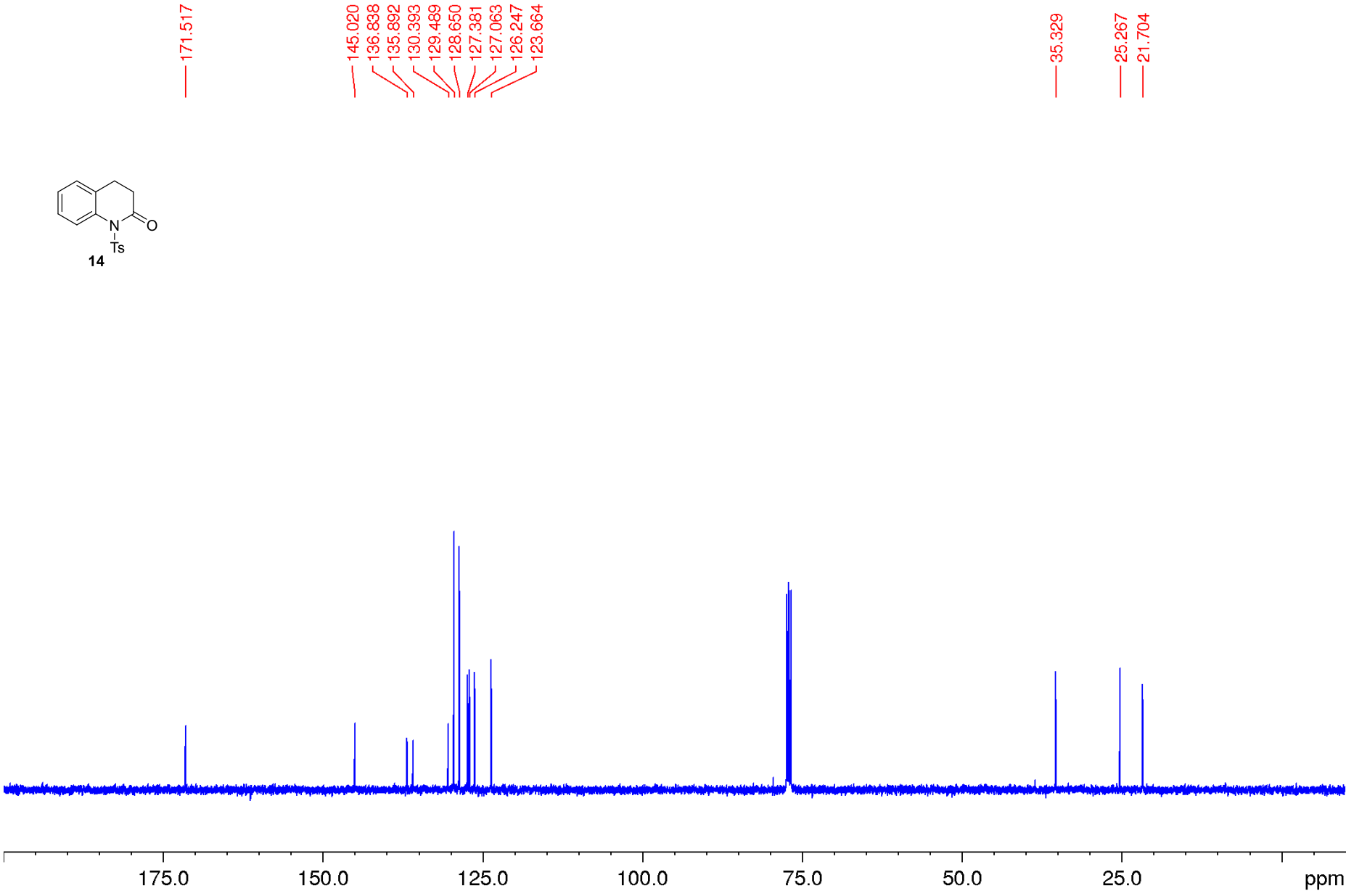
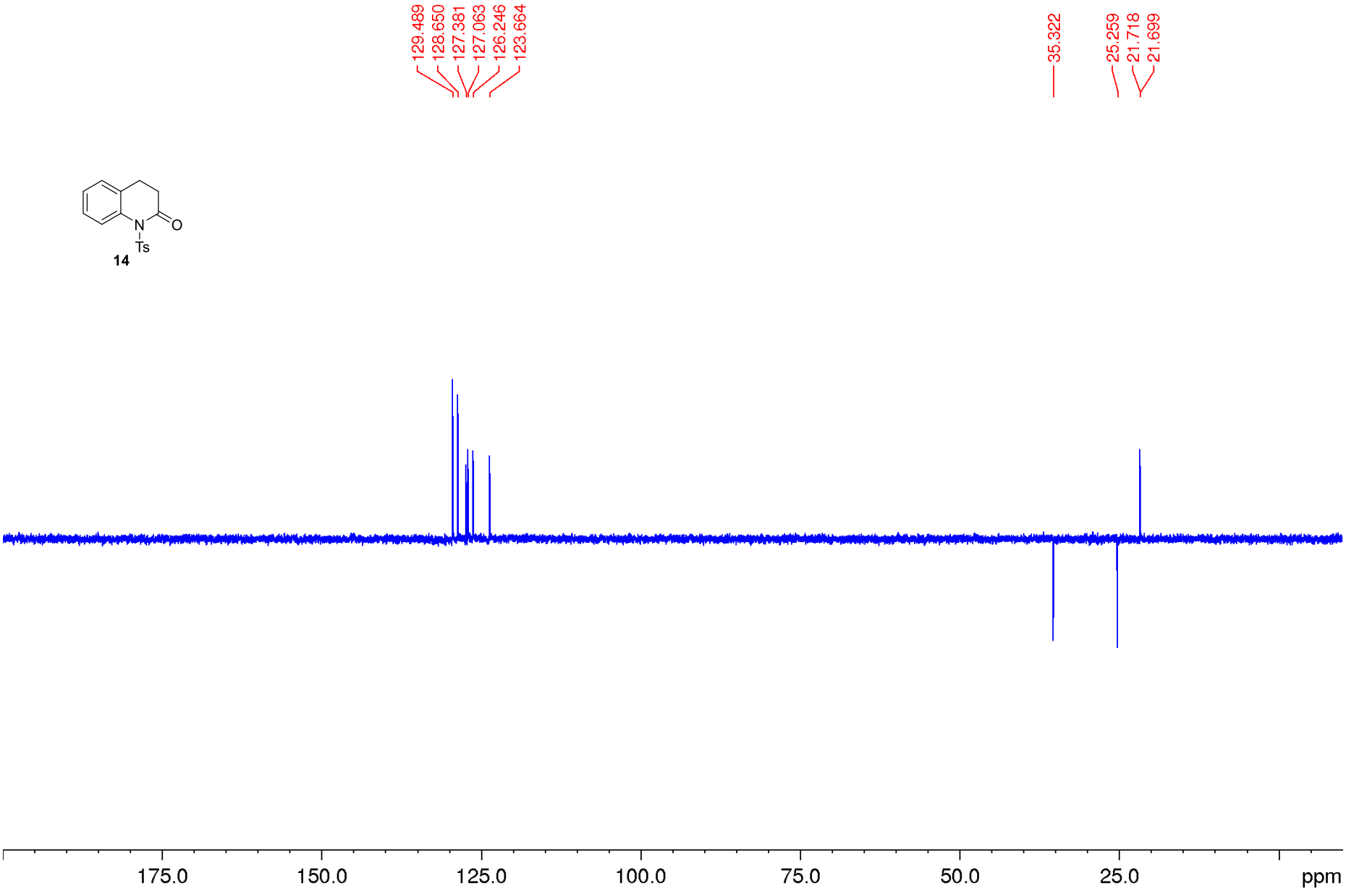
7.756
7.736
7.592
7.572
7.473
7.453
7.279
7.261
7.240
7.211
7.189
7.179
7.159
7.140
7.122
7.108
7.088
7.067
7.049
7.029
6.965
6.946
6.928
6.865
6.846
2.570
2.546
2.510
2.499
2.462
2.456
2.436
2.415
2.407
2.400
2.386
2.374
2.366
2.338
2.329
2.271
NHTs
N
O
Ts
13
7.5
7.0
ppm
2.6
2.4
2.2
2.0
ppm
0.992
1.976
1.000
1.947
1.110
4.192
4.351
1.010
1.002
4.005
4.217
3.007
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

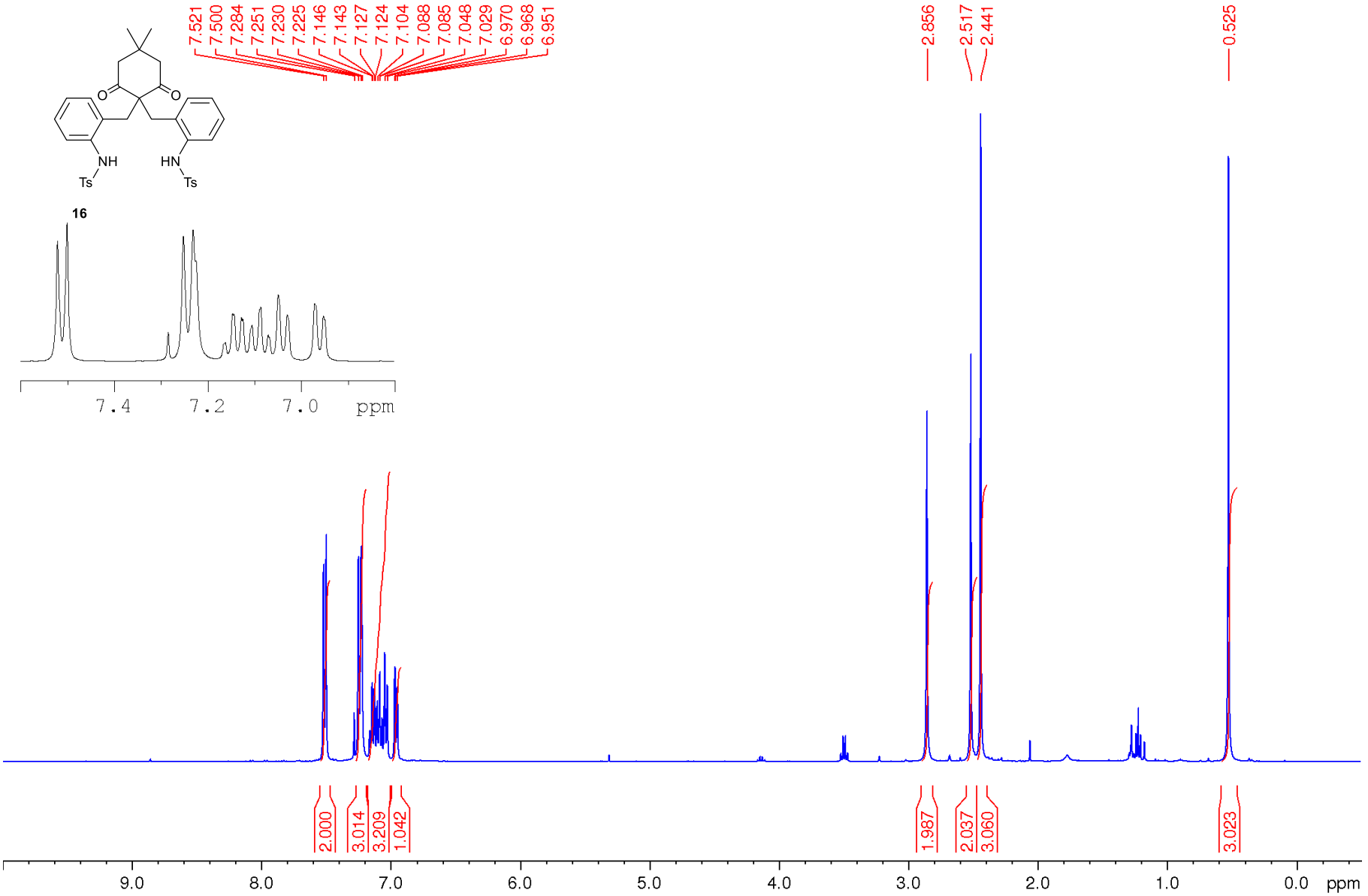

174.367
145.349
143.368
137.262
135.975
134.986
134.808
131.613
131.043
129.556
129.505
129.446
128.666
127.602
127.350
126.998
126.664
125.754
123.898
45.436
30.999
29.765
21.824
21.550
NHTs
N
O
Ts
13
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

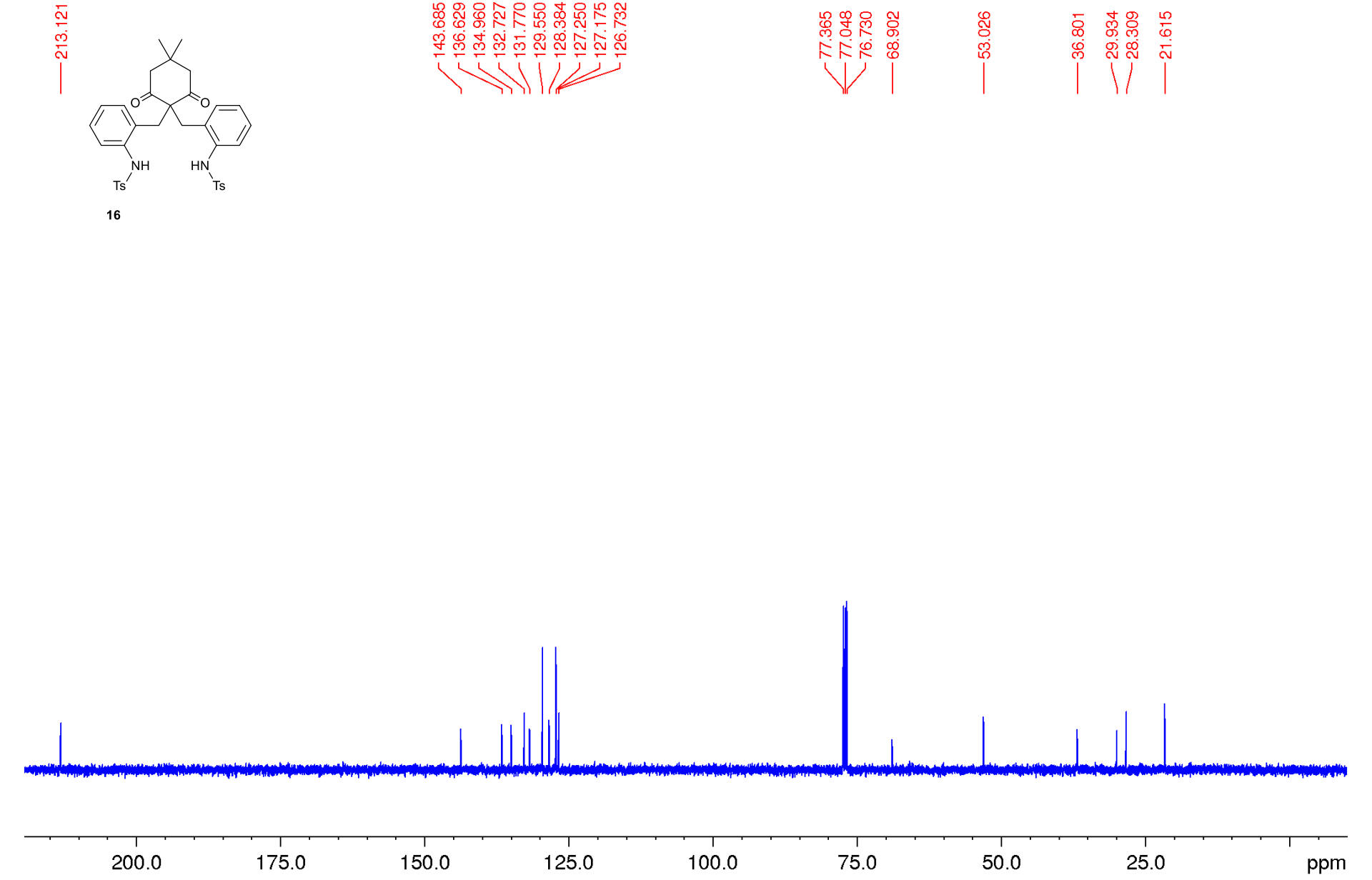

131.043
129.556
129.506
128.666
127.604
127.349
127.000
126.663
125.750
123.898
45.435
31.000
29.763
21.821
21.549
NHTs
N
O
Ts
13
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

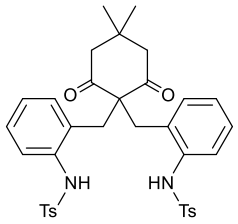

7.876
7.856
7.589
7.569
7.262
7.241
7.215
7.183
7.149
7.131
7.113
2.712
2.697
2.680
2.498
2.481
2.466
2.362
N
O
Ts
14
8.0
7.5
ppm
2.8
2.6
2.4
2.2
ppm
2.000
0.989
5.460
2.122
2.205
3.140
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


171.517
145.020
136.838
135.892
130.393
129.489
128.650
127.381
127.063
126.247
123.664
35.329
25.267
21.704
N
O
Ts
14
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


129.489
128.650
127.381
127.063
126.246
123.664
35.322
25.259
21.718
21.699
N
O
Ts
14
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

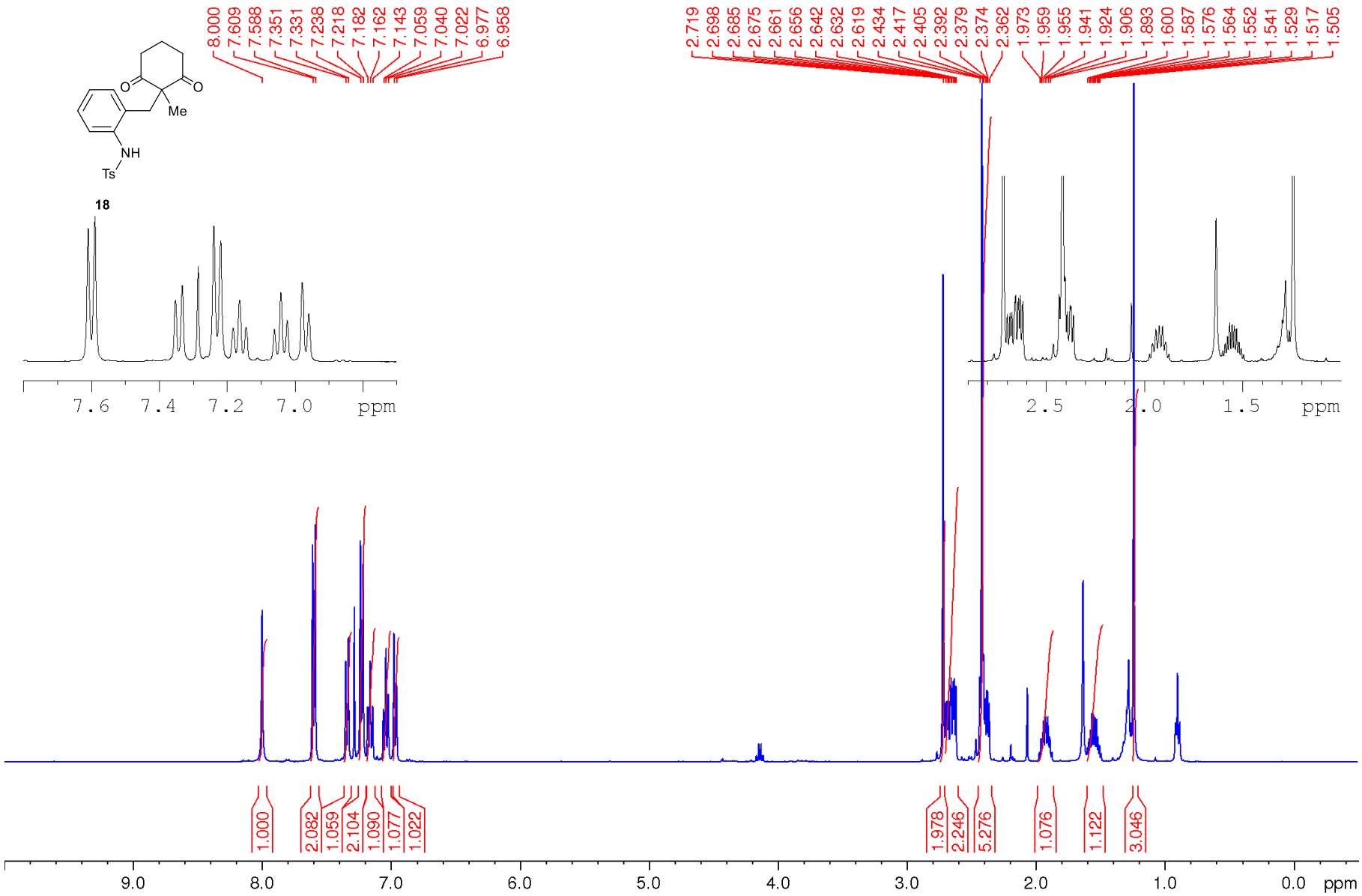

7.521
7.500
7.284
7.251
7.230
7.225
7.146
7.143
7.127
7.124
7.104
7.088
7.085
7.048
7.029
6.970
6.968
6.951
2.856
2.517
2.441
0.525
O
O
NH
Ts
HN
Ts
16
7.4
7.2
7.0
ppm
2.000
3.014
3.209
1.042
1.987
2.037
3.060
3.023
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

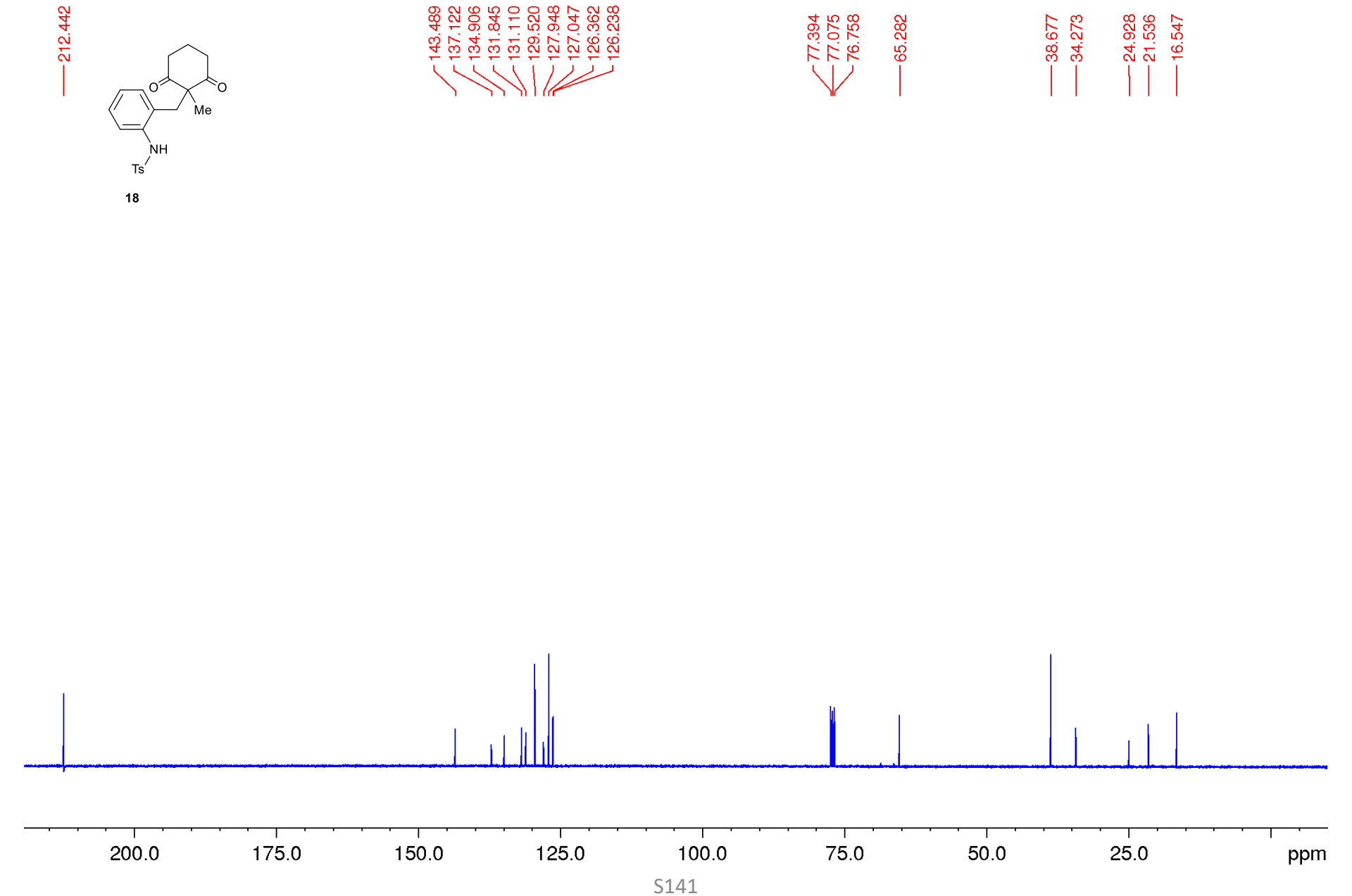

213.121
143.685
136.629
134.960
132.727
131.770
129.550
128.384
127.250
127.175
126.732
77.365
77.048
76.730
68.902
53.026
36.801
29.934
28.309
21.615
O
O
NH
Ts
HN
Ts
16
200.0
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

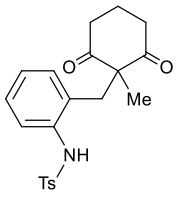

O
O
NH
Ts
HN
Ts

16

132.727
129.549
128.383
127.249
127.174
126.731
53.026
36.802
28.310
21.615
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

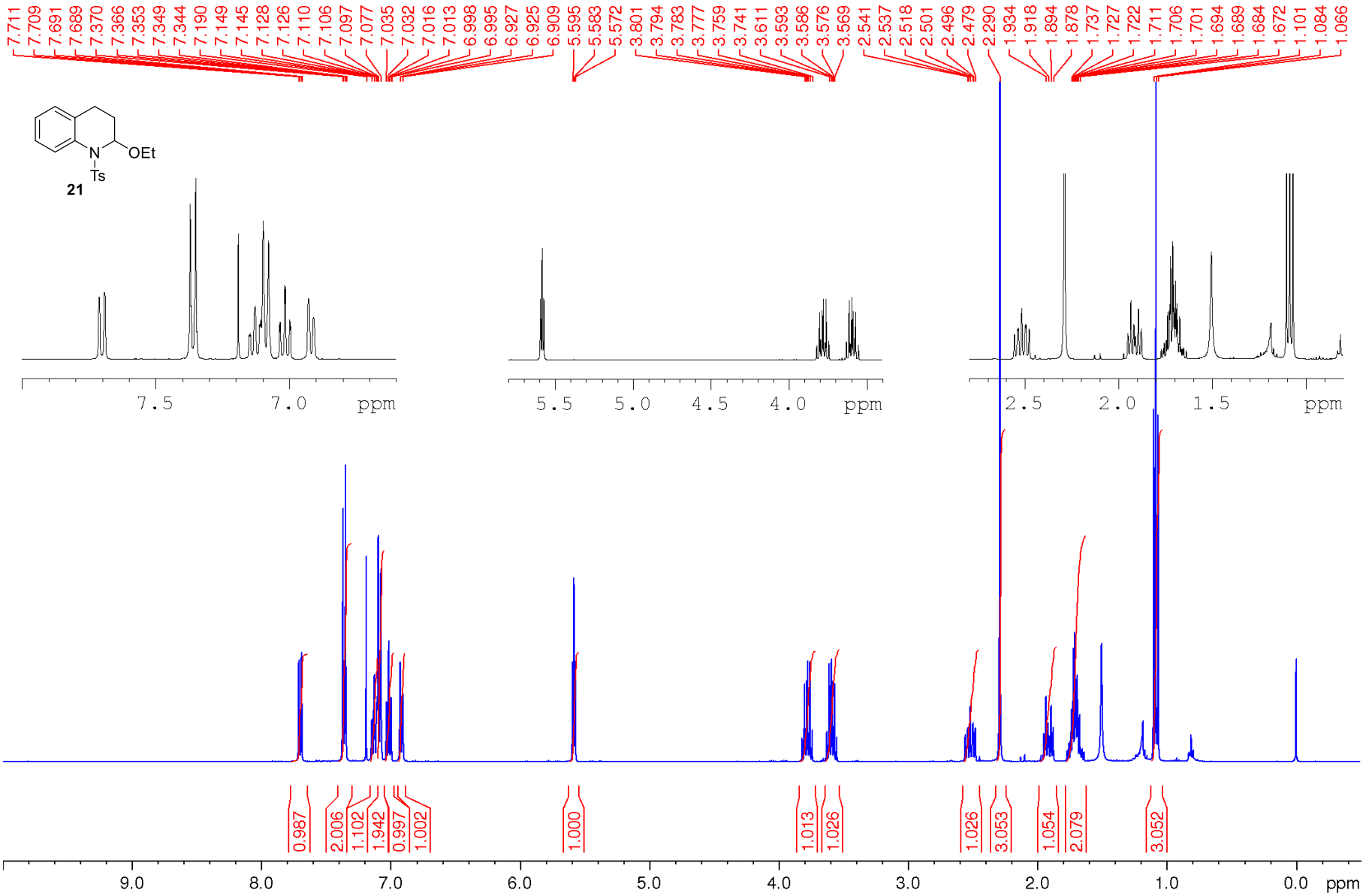

8.000
7.609
7.588
7.351
7.331
7.238
7.218
7.182
7.162
7.143
7.059
7.040
7.022
6.977
6.958
2.719
2.698
2.685
2.675
2.661
2.656
2.642
2.632
2.619
2.434
2.417
2.405
2.392
2.379
2.374
2.362
1.973
1.959
1.955
1.941
1.924
1.906
1.893
1.600
1.587
1.576
1.564
1.552
1.541
1.529
1.517
1.505
O
O
Me
NH
Ts
18
7.6
7.4
7.2
7.0
ppm
2.5
2.0
1.5
ppm
1.000
2.082
1.059
2.104
1.090
1.077
1.022
1.978
2.246
5.276
1.076
1.122
3.046
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


212.442
143.489
137.122
134.906
131.845
131.110
129.520
127.948
127.047
126.362
126.238
77.394
77.075
76.758
65.282
38.677
34.273
24.928
21.536
16.547
O
O
Me
NH
Ts
18
200.0
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


O
O
Me
NH
Ts

18

131.110
129.520
127.947
127.047
126.362
126.238
38.677
34.273
24.929
21.536
16.548
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm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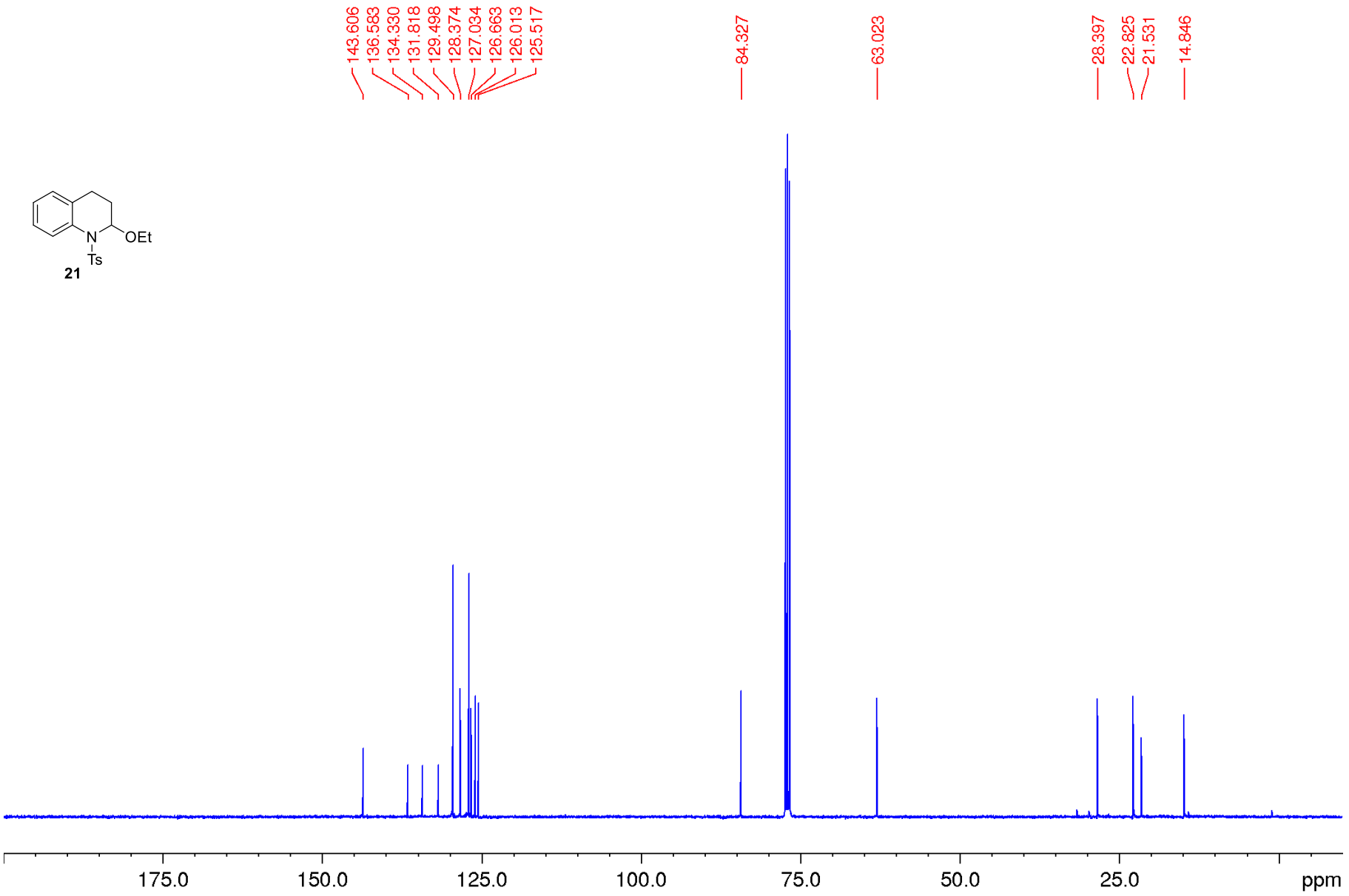
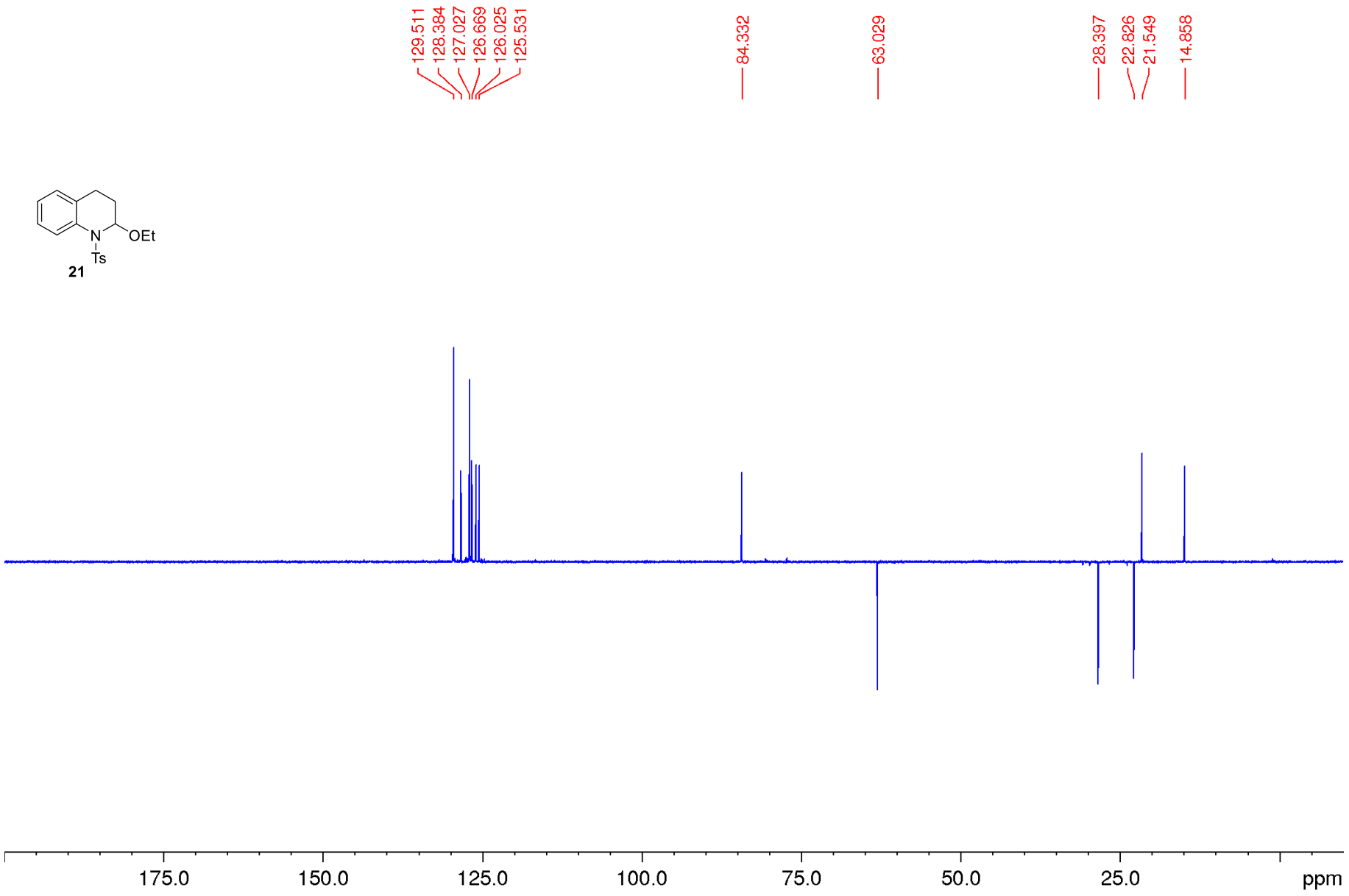
7.709
7.691
7.689
7.370
7.366
7.353
7.349
7.344
7.190
7.149
7.145
7.128
7.126
7.110
7.106
7.097
7.077
7.035
7.032
7.016
7.013
6.998
6.995
6.927
6.925
6.909
5.595
5.583
5.572
3.801
3.794
3.783
3.777
3.759
3.741
3.611
3.593
3.586
3.576
3.569
2.541
2.537
2.518
2.501
2.496
2.479
2.290
1.934
1.918
1.894
1.878
1.737
1.727
1.722
1.711
1.706
1.701
1.694
1.689
1.684
1.672
1.101
1.084
1.066
OEt
N
Ts
21
7.5
7.0
ppm
5.5
5.0
4.5
4.0
ppm
2.5
2.0
1.5
ppm
0.987
2.006
1.102
1.942
0.997
1.002
1.000
1.013
1.026
1.026
3.053
1.054
2.079
3.052
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


143.606
136.583
134.330
131.818
129.498
128.374
127.034
126.663
126.013
125.517
84.327
63.023
28.397
22.825
21.531
14.846
OEt
N
Ts
21
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm


129.511
128.384
127.027
126.669
126.025
125.531
84.332
63.029
28.397
22.826
21.549
14.858
N
Ts
OEt
21
175.0
150.0
125.0
100.0
75.0
50.0
25.0
ppm

2. HF calculations on diastereomers 9 and 10

Calculated by HF/6-31G* in Titan 1.0.1 2000, Wavefunction inc. 18401, Von Karman Ave., Ste. 370, Irvine, CA, 92612.

TRANS 1 (AX-AX)

```
  |  Jaguar version 3.5, release  42
|
  |
|
  |  Copyright 1991-1998 Schrodinger, Inc.
|
  |  All Rights Reserved.
|
  |
|
  |  Use of this program should be acknowledged in publications
as:    |
  |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.
|
  +-----------------------------------------------------------
-----+

  start of program pre
  Job name: WF22668
  Executables used: D:\TITAN
  Temporary files : C:\Users\gfabr\AppData\Local\Temp\WF22668

  Input file comments:
    Molecule001
    This file created by Spartan

  basis set:              6-31G**
  net molecular charge:     0
  multiplicity:             1

  number of basis functions....          370

 Input geometry:
                                  angstroms
  atom            x                   y                   z
  H1         1.1191280000      1.6965320000     -2.2509690000
  C1         1.4327850000      1.6294290000     -1.2024610000
  C2         2.2328070000      1.4713840000      1.4583710000
  C3         0.5926240000      1.0171390000     -0.2715530000
  C4         2.6604480000      2.1504380000     -0.8148190000
  C5         3.0556090000      2.0728000000      0.5161590000
  C6         0.9980480000      0.9291670000      1.0714170000
  C7        -0.7366610000      0.4875910000     -0.7242400000
  H3         3.3127550000      2.6243320000     -1.5552690000
  H4         4.0191110000      2.4912150000      0.8258060000
  H6         2.5602660000      1.4333460000      2.5047160000
  C16       -0.6564400000     -0.9091000000     -1.2872560000
```

```
 C8       -1.7767140000      0.5545650000      0.4065880000
 N2        0.1369600000      0.3291820000      2.0599610000
 C9       -1.2160840000      0.0265430000      1.7187400000
 C11       0.7864030000     -0.3460990000      3.2062420000
 O1       -1.8898630000     -0.5990320000      2.5238060000
 C18      -0.5975730000     -3.4826560000     -2.3750650000
 C19      -1.6868380000     -1.3481750000     -2.1250480000
 C20       0.4028530000     -1.7700630000     -1.0039250000
 C21       0.4309410000     -3.0509710000     -1.5461470000
 C22      -1.6567650000     -2.6278170000     -2.6641050000
 H2       -2.5248140000     -0.6797570000     -2.3561340000
 H5        1.2218680000     -1.4344730000     -0.3558570000
 H7        1.2671570000     -3.7195330000     -1.3164750000
 H8       -2.4691590000     -2.9639050000     -3.3168950000
 H9       -0.5752030000     -4.4915270000     -2.7994430000
 H10      -1.1002520000      1.1510230000     -1.5523860000
 C10      -2.2895290000      1.9731500000      0.6058680000
 H11      -1.4766350000      2.6771600000      0.8283160000
 H12      -3.0098870000      2.0227780000      1.4327030000
 H13      -2.7989650000      2.3360840000     -0.2969260000
 H14      -2.6432040000     -0.0942940000      0.1178860000
 H15       1.7587900000     -0.7715170000      2.9196000000
 H16       0.1662720000     -1.1625360000      3.6017490000
 H17       0.9497620000      0.3775990000      4.0170460000

 Molecular weight:    251.13 amu

 Stoichiometry:        C17NH17O
 Molecular Point Group: C1
 Point Group used: C1
 nuclear repulsion energy.......  1408.065361920 hartrees

Non-default options chosen:
  Geometry will be optimized in redundant internal coordinates
  Initial Hessian: from previous calculation

 end of program pre


 start of program onee
 smallest eigenvalue of S:    3.619E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program hfig
 initial wavefunction generated automatically from atomic
wavefunctions

 Irreducible     Total no   No of occupied orbitals
 representation  orbitals   Shell_1  Shell_2    ...
 No Symm          368         67
```

```
  -------------------------
  Orbital occupation/shell    1.000

  end of program hfig


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom         H1     C1      C2      C3      C4      C5      C6
C7
  grid # 1        72     88      88      90      89      89      87
81
  grid # 2       116     95      96     100      97      97      99
90
  grid # 3       216    183     184     191     184     184     187
173
  grid # 4       223    326     328     338     327     327     329
309

  number of gridpoints:
     atom         H3     H4      H6     C16      C8      N2      C9
C11
  grid # 1        73     73      70      90      82      98      85
73
  grid # 2       118    118     113     100      91     106      94
80
  grid # 3       224    223     209     196     174     218     179
150
  grid # 4       232    232     219     342     310     397     300
283

  number of gridpoints:
     atom         O1    C18     C19     C20     C21     C22      H2
H5
  grid # 1       111     89      88      89      89      89      70
71
  grid # 2       122     97      96      95      97      97     113
111
  grid # 3       260    185     184     183     185     185     214
213
  grid # 4       459    328     328     328     327     328     221
217

  number of gridpoints:
     atom         H7     H8      H9     H10     C10     H11     H12
H13
```

```
  grid # 1       73     73     73     68     73     72     71
71
  grid # 2      118    118    118    107     80    109    111
110
  grid # 3      224    224    224    205    152    218    220
216
  grid # 4      232    232    232    203    297    221    225
221

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       68     71     71     71   2879
  grid # 2      111    109    110    111   3750
  grid # 3      208    213    216    217   7221
  grid # 4      208    219    221    223  10092

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf
 number of electrons.........        134
 number of alpha electrons....        67
 number of beta electrons.....        67
 number of orbitals, total....       368
 number of core orbitals......        67
 number of open shell orbs....         0
 number of occupied orbitals..        67
 number of virtual orbitals...       301
 number of hamiltonians.......         1
 number of shells.............         1
 SCF type: HF

       i  u  d  i  g                                          RMS     maximum
       t  p  i  c  r                              energy   density    DIIS
       e  d  i  u  i                total energy  change   change     error

etot   1  N  N  5  M  -780.39852533395           4.6E-03  1.0E-01
etot   2  Y  Y  6  M  -782.67625085536  2.3E+00  2.0E-03  4.3E-02
etot   3  Y  Y  6  M  -782.93254472020  2.6E-01  9.1E-04  2.3E-02
etot   4  N  Y  2  U  -783.00030881246  6.8E-02  8.7E-04  1.6E-02
etot   5  Y  Y  6  M  -783.01057256373  1.0E-02  1.2E-03  9.2E-03
etot   6  N  Y  2  U  -783.01587000907  5.3E-03  1.3E-04  2.0E-03
etot   7  Y  Y  6  M  -783.01618285999  3.1E-04  5.5E-05  5.5E-04
etot   8  Y  Y  6  M  -783.01624499366  6.2E-05  1.3E-05  1.6E-04
etot   9  N  Y  2  U  -783.01614028065 -1.0E-04  5.8E-06  4.4E-05
etot  10  Y  Y  6  M  -783.01614787467  7.6E-06  3.0E-06  3.8E-05
etot  11  Y  N  6  M  -783.01615200071  4.1E-06  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1408.06536191963
   (E)  Total one-electron terms..... -3860.78785845841
   (I)  Total two-electron terms.....  1669.70634453807
   (L)  Electronic energy..... -2191.08151392033  (E+I)
   (N)  Total energy.............  -783.01615200071  (A+L)

 SCFE: SCF energy: HF    -783.01615200071 hartrees   iterations:
11


 HOMO energy:    -0.30356
 LUMO energy:     0.12736

  Orbital energies:
 -20.52960  -15.60152  -11.35603  -11.28995  -11.26392  -11.25243
 -11.25184  -11.24506  -11.24373  -11.24338  -11.24180  -11.24111
 -11.23660  -11.23531  -11.23528  -11.23458  -11.23264  -11.23175
 -11.22896   -1.37802   -1.24719   -1.16508   -1.14381   -1.10902
  -1.03504   -1.01651   -1.01205   -1.00829   -0.94853   -0.93032
  -0.85617   -0.83967   -0.82837   -0.81815   -0.79129   -0.72886
  -0.70636   -0.69621   -0.66671   -0.64354   -0.63966   -0.63669
  -0.62438   -0.61229   -0.60496   -0.59621   -0.59273   -0.58149
  -0.58042   -0.56346   -0.54466   -0.54100   -0.53137   -0.52118
  -0.51494   -0.50164   -0.49630   -0.49416   -0.48351   -0.46786
  -0.46684   -0.41857   -0.40863   -0.34217   -0.33272   -0.32150
  -0.30356    0.12736    0.13083    0.14229    0.14682    0.19439
   0.22478    0.23269    0.23931    0.25591    0.28182

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1      3.282581E-03  -1.437197E-03   1.418645E-02
   2    C1      2.298364E-03   1.660870E-03   5.083617E-04
   3    C2      1.272136E-03  -1.561267E-03   7.524506E-03
   4    C3      9.983834E-03   1.150637E-02   3.755712E-03
```

```
 5    C4      6.631700E-03   4.472319E-03  -8.542985E-03
 6    C5      6.115223E-03   1.820293E-03   6.730213E-04
 7    C6     -7.835891E-03   2.216502E-03   8.256945E-03
 8    C7     -1.087968E-02   1.111272E-02  -1.206579E-02
 9    H3     -8.150986E-03  -5.736693E-03   9.302946E-03
10    H4     -1.242737E-02  -5.347578E-03  -3.408193E-03
11    H6     -6.730423E-03   3.859971E-04  -1.594048E-02
12    C16     2.460625E-03  -1.147914E-02  -8.256392E-03
13    C8     -1.206907E-02  -9.751302E-03  -6.732659E-03
14    N2     -1.051122E-02  -1.073566E-02  -3.416459E-02
15    C9      1.006629E-02  -2.618310E-02   5.557412E-02
16    C11    -6.139425E-03   4.581737E-04   8.360836E-03
17    O1      1.971210E-02   2.481345E-02  -3.659501E-02
18    C18     1.901707E-03  -8.667953E-03  -2.626967E-03
19    C19    -2.547787E-03  -9.608923E-04  -1.768933E-03
20    C20     5.113784E-03   2.044606E-03   4.667870E-03
21    C21     4.565050E-03  -6.593856E-03   1.128949E-03
22    C22    -7.827781E-03  -1.161037E-03  -4.631446E-03
23    H2      1.089719E-02  -8.112877E-03   2.377892E-03
24    H5     -1.209344E-02  -5.945461E-03  -1.068225E-02
25    H7     -1.036894E-02   8.228927E-03  -2.879715E-03
26    H8      1.013157E-02   4.190342E-03   7.851156E-03
27    H9     -1.683267E-04   1.253218E-02   5.065976E-03
28    H10     6.333236E-03  -1.277191E-02   1.737267E-02
29    C10    -7.306673E-03   1.936632E-02   6.872197E-03
30    H11    -5.950012E-03  -6.201921E-03  -1.674953E-03
31    H12     6.039693E-03  -1.418829E-03  -6.455421E-03
32    H13     4.487222E-03  -4.739483E-03   6.206494E-03
33    H14     1.960896E-02   1.184381E-02   1.360273E-02
34    H15    -1.087916E-02   6.456172E-03  -1.620599E-03
35    H16     2.280555E-03   1.341945E-02  -9.737619E-03
36    H17    -8.009202E-04  -7.383838E-03  -6.482669E-03
-----------   -------------  -------------  -------------
  total       4.947295E-04   3.385128E-04  -9.778370E-04

 end of program der1b


 start of program geopt   1

 geometry optimization step  1
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3001025
  Cos(theta):   0.7853411

  Final level shift:  -6.5014507E-02

 gradient maximum:        4.7648E-02 .  (  4.5000E-04 )
```

```
  gradient rms:            1.0796E-02 .  (  3.0000E-04 )
  step size:   0.30009  trust radius:   0.30000
  displacement maximum:    1.0985E-01 .  (  1.8000E-03 )
  displacement rms:        2.7169E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.6979E-02    geom step:   3.0009E-
01    full step:   3.0009E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.4080E-02     y:    -1.6582E-02     z:    -1.8506E-02

  new geometry:
                              angstroms
  atom            x                y                z
  H1         1.1353843962     1.7223305973    -2.2079059337
  C1         1.4426196492     1.6586199182    -1.1764133383
  C2         2.2139562261     1.5013171305     1.4552317580
  C3         0.6024544405     1.0279713092    -0.2696501528
  C4         2.6607868239     2.1967707846    -0.7949665076
  C5         3.0387672647     2.1174588972     0.5284985945
  C6         0.9979596045     0.9360894155     1.0596198202
  C7        -0.7263094728     0.4665253517    -0.7161776176
  H3         3.2949510662     2.6722927385    -1.5220172409
  H4         3.9762973964     2.5412950672     0.8490357375
  H6         2.5252755444     1.4666683485     2.4835525781
  C16       -0.6533685426    -0.9435012981    -1.3054302903
  C8        -1.7392704779     0.5514602000     0.4459509705
  N2         0.1565755521     0.3112620949     2.0121009287
  C9        -1.1658732764    -0.0035231485     1.7456405927
  C11        0.7319935965    -0.2551595532     3.2300681698
  O1        -1.8539771807    -0.6179011441     2.5119308218
  C18       -0.6338807008    -3.5116796189    -2.4149530757
  C19       -1.6828353543    -1.3638909216    -2.1522312536
  C20        0.3814193524    -1.8313670938    -1.0265774784
  C21        0.3937314261    -3.1063920781    -1.5749919114
  C22       -1.6795471828    -2.6305191551    -2.7027460817
  H2        -2.4839389746    -0.6851904202    -2.3957909383
  H5         1.1793485050    -1.5359512811    -0.3750516125
  H7         1.1978965669    -3.7867494531    -1.3394806061
  H8        -2.4705584338    -2.9315777960    -3.3660729058
  H9        -0.6231073850    -4.4970564258    -2.8468134047
  H10       -1.1072456665     1.1151086627    -1.5005994737
  C10       -2.2542140462     1.9850940657     0.6783426550
  H11       -1.4441938227     2.6806779486     0.8760642846
  H12       -2.9352733731     2.0107724942     1.5224806907
  H13       -2.7872119916     2.3287805408    -0.2022175894
  H14       -2.5869666576    -0.0884850835     0.2355433692
  H15        1.7072167409    -0.6857481520     2.9916283960
  H16        0.0570160348    -1.0141469039     3.6144880619
  H17        0.8658888111     0.5142404534     4.0024593104

  nuclear repulsion energy.......  1410.701731739 hartrees
```

```
  ------------------------------------------------
 /  end of geometry optimization iteration   1   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.360E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     86     89     92     89     89     84
81
  grid # 2      116     95     95    100     97     97     94
91
  grid # 3      216    182    184    193    182    182    188
172
  grid # 4      215    326    328    339    326    326    326
316

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     70     90     82     95     82
70
  grid # 2      118    118    113    100     90    106     92
80
  grid # 3      223    223    210    197    174    215    176
148
  grid # 4      224    223    209    342    312    392    296
274

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     95     97     97    113
112
  grid # 3      260    185    183    183    185    183    213
212
```

```
  grid # 4      455    330    327    327    329    330    214
210

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     69     73     72     71
71
  grid # 2      118    118    118    105     80    110    111
110
  grid # 3      223    223    224    203    149    218    219
216
  grid # 4      224    224    224    201    287    216    220
217

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     71     71   2871
  grid # 2      109    108    106    111   3735
  grid # 3      212    213    214    217   7200
  grid # 4      206    219    213    224   9971

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                          RMS    maximum
      t  p  i  c  r                          energy  density   DIIS
      e  d  i  u  i                          change  change    error
      r  t  s  t  d     total energy

etot  1  N  N  2  U  -783.01938171043                  3.1E-04  7.1E-03
etot  2  Y  Y  6  M  -783.03000043113  1.1E-02  1.1E-04  2.1E-03
etot  3  N  Y  2  U  -783.03106344985  1.1E-03  3.7E-05  7.6E-04
etot  4  Y  Y  6  M  -783.03119881510  1.4E-04  1.7E-05  2.6E-04
etot  5  Y  Y  6  M  -783.03121880962  2.0E-05  5.7E-06  8.9E-05
etot  6  Y  Y  6  M  -783.03122607122  7.3E-06  2.7E-06  3.2E-05
etot  7  Y  N  6  M  -783.03122787331  1.8E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1410.70173173934
   (E)  Total one-electron terms..... -3865.92950785311
   (I)  Total two-electron terms.....  1672.19654824046
   (L)  Electronic energy............. -2193.73295961265  (E+I)
   (N)  Total energy.................  -783.03122787331  (A+L)
```

```
 SCFE: SCF energy: HF    -783.03122787331 hartrees   iterations:
7


 HOMO energy:    -0.30459
 LUMO energy:     0.13091

  Orbital energies:
 -20.52749  -15.60051  -11.34642  -11.28806  -11.25842  -11.24930
 -11.24169  -11.24151  -11.24092  -11.23985  -11.23904  -11.23689
 -11.23258  -11.23159  -11.23058  -11.23024  -11.22970  -11.22775
 -11.22403   -1.39461   -1.26592   -1.16468   -1.14858   -1.10594
  -1.03237   -1.01829   -1.01747   -1.01191   -0.95489   -0.93254
  -0.85685   -0.84724   -0.83382   -0.82046   -0.79637   -0.73948
  -0.70805   -0.69963   -0.67024   -0.64928   -0.64673   -0.63613
  -0.63148   -0.61408   -0.61049   -0.59856   -0.59365   -0.58456
  -0.57983   -0.56458   -0.55067   -0.54504   -0.53493   -0.52320
  -0.51862   -0.50614   -0.49931   -0.49565   -0.48542   -0.46889
  -0.46589   -0.42132   -0.40774   -0.34161   -0.33299   -0.32094
  -0.30459    0.13091    0.13291    0.14430    0.14764    0.20850
   0.23002    0.23762    0.24562    0.25861    0.28796

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

 atom  label          x             y             z
 ----  -----   -------------  -------------  -------------
   1    H1     -1.514374E-04  -3.096039E-04   1.002164E-03
   2    C1      1.301644E-03   8.729967E-04  -1.861714E-03
   3    C2     -3.657433E-04  -2.143944E-03   6.648631E-04
   4    C3      2.594005E-03   2.719820E-03  -5.723392E-03
   5    C4     -3.147285E-03  -5.528582E-04  -5.309929E-03
   6    C5      1.162814E-03  -8.982218E-04   4.857120E-03
   7    C6     -9.638467E-04   5.275631E-03   8.866151E-03
   8    C7     -4.730814E-03  -6.001486E-04   1.334736E-03
   9    H3     -2.777231E-04   2.306371E-05   2.461452E-04
  10    H4     -1.426506E-03  -7.724899E-04   5.474090E-04
  11    H6     -1.770156E-03  -3.865938E-04  -9.211702E-04
  12    C16     9.943502E-04  -2.424272E-03  -7.414661E-04
  13    C8      3.149883E-04  -2.131484E-03   3.380947E-03
```

```
 14    N2     -7.793412E-03  -1.374417E-02   4.559268E-04
 15    C9      4.333499E-03   9.066313E-03  -4.723013E-03
 16    C11     5.234472E-03   5.077006E-03   4.690626E-03
 17    O1      4.760130E-03   1.883641E-03  -1.121553E-03
 18    C18    -2.270831E-03   5.018101E-03   5.055633E-04
 19    C19     3.256554E-03   1.223243E-03   5.902529E-04
 20    C20    -4.280619E-03   1.916285E-03   1.891580E-04
 21    C21    -5.265252E-03  -2.993652E-03  -2.766635E-03
 22    C22     8.589172E-03  -5.527471E-03   1.497082E-03
 23    H2      8.052200E-05   3.648249E-05   8.471907E-04
 24    H5      2.111037E-03   1.310376E-03   4.538936E-04
 25    H7     -1.409030E-03   2.194106E-03  -8.314943E-04
 26    H8     -6.462185E-04  -3.620992E-04   2.889795E-04
 27    H9     -2.881855E-04   5.095360E-05   1.073475E-04
 28    H10     8.607824E-04  -8.939108E-04  -5.707014E-04
 29    C10     2.047501E-03  -1.760007E-03   1.143945E-03
 30    H11    -1.816107E-04  -7.393073E-04  -4.973610E-04
 31    H12    -1.006128E-04  -4.610591E-04  -7.477742E-04
 32    H13    -2.027130E-04   2.866088E-04   6.346529E-05
 33    H14    -1.253089E-05   1.213578E-03  -5.111228E-04
 34    H15    -6.434327E-03   4.048267E-04   3.576926E-03
 35    H16     5.186746E-03   4.318448E-03  -3.489497E-03
 36    H17    -8.137023E-04  -6.008042E-03  -6.129437E-03
-----------   ------------   ------------   ------------
   total       2.956614E-04   1.821400E-04  -6.363694E-04

 end of program der1b


 start of program geopt   2

 geometry optimization step  2
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3000331
  Cos(theta):   0.4305863

  Final level shift:  -1.2795320E-02

 energy change:          -1.5076E-02 .  (  5.0000E-05 )
 gradient maximum:        1.0864E-02 .  (  4.5000E-04 )
 gradient rms:            2.9859E-03 .  (  3.0000E-04 )
 step size:   0.30000  trust radius:   0.30000
 displacement maximum:    1.5538E-01 .  (  1.8000E-03 )
 displacement rms:        2.7161E-02 .  (  1.2000E-03 )
 predicted energy change:    -2.7061E-03    geom step:   3.0000E-
01    full step:   3.0000E-01
 molecular structure not yet converged...
```

```
 center of mass moved by:
    x:     1.2165E-03     y:    -1.3489E-02     z:    -1.8772E-02

 new geometry:
                                angstroms
 atom            x                  y                  z
 H1         1.1193905048       1.8126267842      -2.2034859292
 C1         1.4308984614       1.7248948198      -1.1786423510
 C2         2.1967769756       1.4819080132       1.4630351635
 C3         0.5976680706       1.0602449623      -0.2878106471
 C4         2.6419529465       2.2575457752      -0.7762343401
 C5         3.0154115602       2.1337516344       0.5539877031
 C6         0.9912258814       0.9228159075       1.0487868998
 C7        -0.7323826996       0.4842551694      -0.7367323528
 H3         3.2763432977       2.7636317489      -1.4812812189
 H4         3.9449226467       2.5529696095       0.8946852948
 H6         2.5015762085       1.4165566260       2.4874633974
 C16       -0.6475858097      -0.9336658601      -1.3146481354
 C8        -1.7324711129       0.5691443353       0.4365301301
 N2         0.1698490065       0.2165844193       1.9564669191
 C9        -1.1501283704      -0.0262040558       1.7065386369
 C11        0.7187310243      -0.2620814101       3.2244322539
 O1        -1.8293686969      -0.6551586097       2.4622106244
 C18       -0.6506913293      -3.5337795940      -2.3621237847
 C19       -1.6775836093      -1.3787597308      -2.1489544407
 C20        0.3838374582      -1.8122171827      -1.0227490006
 C21        0.3736573294      -3.1042118375      -1.5371789164
 C22       -1.6781965342      -2.6608898499      -2.6713098988
 H2        -2.4888559173      -0.7109151224      -2.3922423575
 H5         1.2078174026      -1.4940238389      -0.3928714474
 H7         1.1816049054      -3.7687343674      -1.2896467243
 H8        -2.4849779963      -2.9810785100      -3.3155173957
 H9        -0.6519884895      -4.5305111207      -2.7655035004
 H10       -1.1144608468       1.1175830201      -1.5274628212
 C10       -2.1998504032       2.0116918183       0.7130616652
 H11       -1.3654845606       2.6683152082       0.9454418804
 H12       -2.8947985803       2.0276883032       1.5426087712
 H13       -2.7091364224       2.4089000751      -0.1601924396
 H14       -2.5983685191      -0.0378972304       0.2219087802
 H15        1.6961747392      -0.7060623531       3.0464605562
 H16        0.0381610968      -1.0000343566       3.6137870212
 H17        0.8289224752       0.5379766839       3.9573493264

 nuclear repulsion energy.......  1414.036299556 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   2   /
------------------------------------------------

 end of program geopt


 start of program onee
```

```
  smallest eigenvalue of S:    3.408E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     89     90     89     88     85
81
  grid # 2      116     95     95     98     97     97     93
91
  grid # 3      216    181    183    195    183    183    195
172
  grid # 4      215    326    327    336    327    327    325
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     70     88     82     96     81
68
  grid # 2      118    118    112     98     90    106     91
79
  grid # 3      224    223    208    193    174    211    176
148
  grid # 4      224    223    208    339    311    387    293
278

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     88     87     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      258    183    183    182    184    184    213
211
  grid # 4      454    328    326    326    327    328    214
208

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     71     72     71
71
```

```
  grid # 2      118    118    118    106     79    109    110
110
  grid # 3      223    222    223    204    154    216    220
217
  grid # 4      223    224    224    199    289    216    218
218

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2857
  grid # 2      109    110    106    111   3728
  grid # 3      212    214    212    217   7197
  grid # 4      206    217    209    224   9938

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

        i  u  d  i  g                                          RMS    maximum
        t  p  i  c  r                              energy   density   DIIS
        e  d  i  u  i                 total energy change   change    error

etot    1  N  N  2  U  -783.02136155277          2.8E-04  7.8E-03
etot    2  Y  Y  6  M  -783.03136759458  1.0E-02 1.1E-04  1.8E-03
etot    3  N  Y  2  U  -783.03248252720  1.1E-03 3.2E-05  5.2E-04
etot    4  Y  Y  6  M  -783.03256116563  7.9E-05 1.5E-05  2.4E-04
etot    5  Y  Y  6  M  -783.03258090874  2.0E-05 5.2E-06  9.1E-05
etot    6  Y  Y  6  M  -783.03258545250  4.5E-06 3.8E-06  6.2E-05
etot    7  Y  N  6  M  -783.03258773896  2.3E-06 0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.03629955572
   (E)  Total one-electron terms..... -3872.60797626611
   (I)  Total two-electron terms.....  1675.53908897143
   (L)  Electronic energy............. -2197.06888729467  (E+I)
   (N)  Total energy.................  -783.03258773896  (A+L)

 SCFE: SCF energy: HF    -783.03258773896 hartrees   iterations:
7


 HOMO energy:    -0.30321
 LUMO energy:     0.13156

  Orbital energies:
```

```
 -20.52271  -15.60097  -11.34219  -11.28805  -11.25738  -11.24922
 -11.24267  -11.24059  -11.24054  -11.23997  -11.23928  -11.23613
 -11.23143  -11.23091  -11.22963  -11.22928  -11.22762  -11.22696
 -11.22393   -1.39739   -1.26887   -1.16423   -1.14847   -1.10634
  -1.03172   -1.02031   -1.01666   -1.01040   -0.95996   -0.93278
  -0.85756   -0.84834   -0.83317   -0.82069   -0.79468   -0.74185
  -0.70968   -0.69922   -0.66980   -0.65048   -0.64746   -0.63565
  -0.62992   -0.61550   -0.61026   -0.60090   -0.59601   -0.58197
  -0.57938   -0.56460   -0.55046   -0.54455   -0.53594   -0.52365
  -0.51980   -0.50645   -0.49936   -0.49482   -0.48499   -0.46893
  -0.46460   -0.42130   -0.40760   -0.34172   -0.33094   -0.32285
  -0.30321    0.13156    0.13367    0.14474    0.14973    0.21032
   0.23174    0.23805    0.24631    0.26000    0.28816

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -3.911478E-04   3.542709E-04  -1.458379E-03
  2    C1     -3.119551E-03  -2.225066E-03   3.531209E-03
  3    C2      6.108036E-04  -1.335699E-04  -2.602108E-03
  4    C3      9.008492E-04  -1.172471E-03  -5.213856E-04
  5    C4      1.225817E-03  -3.332497E-04   4.683335E-03
  6    C5     -1.170997E-03   5.146213E-04  -2.301552E-03
  7    C6     -2.109809E-03   2.064048E-03  -2.254050E-03
  8    C7      1.202640E-03  -1.462120E-03   1.593030E-03
  9    H3      1.815989E-04   1.813854E-05   1.797177E-04
 10    H4      5.309109E-04   2.040217E-04   2.340563E-04
 11    H6      5.591363E-04  -3.274693E-04   1.369180E-03
 12    C16    -3.956222E-03   8.520568E-04  -3.772113E-04
 13    C8      2.454950E-03   1.921568E-03  -3.590774E-04
 14    N2      8.641515E-03   3.070433E-03   3.945689E-03
 15    C9     -1.581657E-03   1.060236E-03  -7.351345E-03
 16    C11     3.887874E-03   3.595520E-04  -2.895027E-03
 17    O1     -7.229827E-03  -2.666916E-03   6.016554E-03
 18    C18     2.917910E-03  -4.248849E-04   1.383904E-03
 19    C19     1.005349E-03   1.404747E-03   6.905326E-04
 20    C20     4.465907E-03  -7.307126E-04   3.099259E-03
 21    C21     2.671215E-03   6.395676E-04   7.848725E-04
```

```
 22    C22    -5.426351E-03   3.024308E-03  -1.345252E-03
 23    H2      7.483926E-04  -1.820965E-04   1.225187E-04
 24    H5     -5.866640E-03  -2.954842E-03  -4.533655E-03
 25    H7      4.726412E-04  -1.123519E-03  -2.027003E-04
 26    H8      2.496669E-03   1.700077E-03   2.002181E-03
 27    H9      9.659810E-04  -5.886098E-04   5.900492E-04
 28    H10    -8.084433E-04   1.599311E-03  -1.592116E-03
 29    C10     2.653684E-03  -1.534465E-03  -1.567911E-03
 30    H11    -1.646321E-03  -7.872101E-04  -3.019026E-04
 31    H12    -5.418789E-04  -6.126750E-05   1.355192E-03
 32    H13     4.762809E-04  -1.678403E-04   1.839367E-04
 33    H14    -1.738107E-03  -7.635143E-04  -6.480034E-04
 34    H15    -3.793343E-03   3.010100E-04   1.341307E-03
 35    H16     1.814264E-03  -8.796190E-05   4.732089E-04
 36    H17    -1.445406E-03  -1.080757E-03  -3.829907E-03
-----------   -------------  -------------  -------------
   total       5.868559E-05   2.794237E-04  -5.618487E-04

 end of program der1b


 start of program geopt   3

 geometry optimization step  3
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:          -1.3599E-03 .  (  5.0000E-05 )
 gradient maximum:        9.3336E-03 .  (  4.5000E-04 )
 gradient rms:            2.3259E-03 .  (  3.0000E-04 )
 step size:   0.28372  trust radius:   0.30000
 displacement maximum:    1.1809E-01 .  (  1.8000E-03 )
 displacement rms:        2.5687E-02 .  (  1.2000E-03 )
 predicted energy change:    -1.3001E-03    geom step:   2.8372E-
01    full step:   2.8372E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:    -7.2246E-03     y:     2.3951E-02     z:     1.5525E-02

 new geometry:
                              angstroms
 atom            x                y                z
 H1        1.0511254407     1.8828349434    -2.2098008415
 C1        1.3844660508     1.7631921226    -1.1932136842
 C2        2.2137248961     1.4247722195     1.4189406178
 C3        0.5738065089     1.0731536158    -0.3052785512
 C4        2.6050670365     2.2794606197    -0.7996036799
 C5        3.0133828284     2.1036429665     0.5137247867
```

```
 C6        0.9920081704      0.9020907964      1.0196384971
 C7       -0.7570698752      0.4875136275     -0.7342452600
 H3        3.2234621656      2.8109208711     -1.5013044160
 H4        3.9542698025      2.4999681140      0.8467527790
 H6        2.5454886850      1.3084361207      2.4313952270
 C16      -0.6553964375     -0.9362424062     -1.2872359414
 C8       -1.7459533021      0.5813579391      0.4434427077
 N2        0.1869515156      0.1782100299      1.9266293327
 C9       -1.1613140564      0.0178953184      1.7195581261
 C11       0.7654927316     -0.3712528435      3.1292554921
 O1       -1.8650251785     -0.5122746065      2.5311817588
 C18      -0.5948449715     -3.5386568700     -2.3177086890
 C19      -1.6235278809     -1.3710197421     -2.1967843737
 C20       0.3338078044     -1.8299689378     -0.9076806346
 C21       0.3655501308     -3.1205758693     -1.4154162473
 C22      -1.5923512076     -2.6553954013     -2.7112899451
 H2       -2.4050327749     -0.6903282694     -2.5060218772
 H5        1.0861203443     -1.5310041441     -0.2174182961
 H7        1.1504935859     -3.7966165663     -1.1031859835
 H8       -2.3355289943     -2.9564896780     -3.4207419947
 H9       -0.5610855132     -4.5373847305     -2.7111691858
 H10      -1.1466239082      1.1075018083     -1.5363412097
 C10      -2.2198012817      2.0168648722      0.7022394019
 H11      -1.3952674756      2.6807594931      0.9306597319
 H12      -2.9210176122      2.0378742470      1.5288404672
 H13      -2.7256179734      2.4030801686     -0.1758784417
 H14      -2.6104846130     -0.0339342616      0.2396894472
 H15       1.6672568851     -0.8988039536      2.8780089012
 H16       0.0580314161     -1.0633791257      3.5643932036
 H17       0.9916607888      0.4003749077      3.8403786522

 nuclear repulsion energy.......  1417.356122328 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   3   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.362E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
```

atom	H1	C1	C2	C3	C4	C5	C6	C7
grid # 1	72	85	88	88	89	87	85	81
grid # 2	116	95	95	98	97	97	93	91
grid # 3	216	182	183	195	183	183	191	173
grid # 4	215	326	326	336	326	327	323	314

number of gridpoints:

atom	H3	H4	H6	C16	C8	N2	C9	C11
grid # 1	73	73	71	88	81	96	81	70
grid # 2	118	118	111	98	90	106	90	79
grid # 3	224	223	207	193	174	209	176	141
grid # 4	224	223	207	340	310	391	291	271

number of gridpoints:

atom	O1	C18	C19	C20	C21	C22	H2	H5
grid # 1	111	89	88	87	89	89	70	71
grid # 2	122	97	96	96	97	97	113	111
grid # 3	260	184	182	182	184	185	214	210
grid # 4	454	329	327	326	327	329	214	207

number of gridpoints:

atom	H7	H8	H9	H10	C10	H11	H12	H13
grid # 1	73	73	73	68	73	72	71	71
grid # 2	118	118	118	105	80	107	109	110
grid # 3	223	223	223	202	148	218	219	217
grid # 4	223	223	224	199	287	215	220	219

number of gridpoints:

atom	H14	H15	H16	H17	total
grid # 1	68	71	70	71	2856
grid # 2	109	109	108	111	3723
grid # 3	214	215	212	216	7184

```
  grid # 4      207    210    209    213   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  2  U  -783.00228408865                3.8E-04  1.7E-02
etot  2  Y  Y  6  M  -783.02874444396  2.6E-02  1.7E-04  7.0E-03
etot  3  N  Y  2  U  -783.03227748154  3.5E-03  4.8E-05  1.7E-03
etot  4  Y  Y  6  M  -783.03246002276  1.8E-04  2.1E-05  6.5E-04
etot  5  Y  Y  6  M  -783.03250696626  4.7E-05  7.4E-06  1.7E-04
etot  6  Y  Y  6  M  -783.03250893662  2.0E-06  3.9E-06  4.7E-05
etot  7  Y  N  6  M  -783.03251144614  2.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1417.35612232773
   (E)  Total one-electron terms..... -3879.18383643504
   (I)  Total two-electron terms.....  1678.79520266117
   (L)  Electronic energy............. -2200.38863377386  (E+I)
   (N)  Total energy.................  -783.03251144614  (A+L)

 SCFE: SCF energy: HF    -783.03251144614 hartrees   iterations:
7


 HOMO energy:    -0.30304
 LUMO energy:     0.13163

  Orbital energies:
  -20.52323  -15.60007  -11.34354  -11.28636  -11.25311  -11.24882
  -11.24231  -11.24039  -11.23995  -11.23977  -11.23915  -11.23544
  -11.23151  -11.23120  -11.23021  -11.22992  -11.22786  -11.22521
  -11.22254   -1.39584   -1.27111   -1.16547   -1.14922   -1.10810
   -1.03304   -1.02111   -1.01747   -1.01184   -0.96268   -0.93323
   -0.85859   -0.84777   -0.83477   -0.82009   -0.79649   -0.74235
   -0.71159   -0.70109   -0.67092   -0.65160   -0.64888   -0.63666
   -0.63338   -0.61565   -0.61139   -0.60290   -0.59761   -0.58403
   -0.58100   -0.56501   -0.54888   -0.54480   -0.53530   -0.52420
   -0.52070   -0.50674   -0.49825   -0.49699   -0.48529   -0.47024
   -0.46449   -0.42026   -0.40868   -0.34208   -0.33226   -0.32309
   -0.30304    0.13163    0.13538    0.14326    0.14990    0.20792
```

```
   0.23153    0.23816    0.24334    0.25969    0.28849

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	3.799907E-05	2.062855E-04	-1.247186E-04
2	C1	-3.320137E-03	-1.950448E-03	1.416294E-03
3	C2	2.083693E-03	9.075049E-04	-3.035847E-04
4	C3	-1.030277E-03	-1.681619E-03	1.459372E-03
5	C4	3.033151E-03	7.064342E-04	4.143072E-03
6	C5	-1.081896E-03	6.804474E-04	-2.681428E-03
7	C6	-1.093058E-03	-9.825934E-04	-3.817772E-03
8	C7	2.456655E-03	5.204630E-04	-3.528671E-04
9	H3	2.131225E-05	-3.678057E-04	4.942864E-04
10	H4	1.434530E-03	6.684642E-04	-7.152819E-06
11	H6	9.000633E-04	3.967989E-04	5.066154E-04
12	C16	-5.094192E-03	-3.741490E-04	-2.257058E-03
13	C8	1.887811E-03	9.008849E-04	-3.067275E-03
14	N2	-6.813761E-03	3.565887E-03	-1.100561E-02
15	C9	1.065183E-03	-6.345649E-04	3.107854E-03
16	C11	-4.787900E-03	-6.917445E-03	1.942500E-03
17	O1	-1.738129E-03	-2.271998E-03	1.886762E-03
18	C18	-1.365493E-04	1.026462E-03	-2.337893E-04
19	C19	1.563066E-03	2.162486E-03	1.193534E-03
20	C20	-2.794822E-03	-2.288840E-03	-2.668097E-03
21	C21	1.773944E-03	-2.261093E-03	6.512729E-04
22	C22	3.106803E-03	2.025543E-03	2.900126E-03
23	H2	2.224789E-03	-2.038599E-03	3.295646E-04
24	H5	5.982254E-03	2.695950E-03	4.409923E-03
25	H7	-3.332877E-03	2.559779E-03	-1.225273E-03
26	H8	-2.893769E-03	-2.175187E-03	-2.232603E-03
27	H9	-8.705405E-04	-1.086142E-03	-1.197889E-03
28	H10	-4.367709E-04	-2.823101E-04	2.448018E-04
29	C10	-2.118518E-03	8.937653E-04	-1.680658E-04
30	H11	8.753990E-04	7.137019E-04	4.823823E-04
31	H12	5.533371E-04	-1.694544E-04	3.171498E-04
32	H13	-2.950149E-04	3.314720E-04	-7.947972E-04
33	H14	-1.089318E-03	-6.201773E-04	-3.886202E-05

```
 34    H15     6.611949E-03  -2.922418E-03  -2.085480E-04
 35    H16     1.849884E-03   3.197009E-03  -9.394257E-04
 36    H17     1.556327E-03   4.847232E-03   7.214890E-03
-----------   -------------  -------------  -------------
   total       9.062102E-05  -1.827433E-05  -6.244174E-04

 end of program der1b


 start of program geopt   4

 geometry optimization step  4
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:           7.6293E-05 .  (  5.0000E-05 )
 gradient maximum:        9.5257E-03 .  (  4.5000E-04 )
 gradient rms:            2.2442E-03 .  (  3.0000E-04 )
 step size:   0.22589  trust radius:   0.30000
 displacement maximum:    1.0732E-01 .  (  1.8000E-03 )
 displacement rms:        2.0451E-02 .  (  1.2000E-03 )
 predicted energy change:    -1.2400E-03    geom step:   2.2589E-
01    full step:   2.2589E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:     4.7253E-03     y:    -1.3031E-02     z:    -3.8420E-03

 new geometry:
                              angstroms
 atom            x                y                z
 H1        1.1070761932     1.8195912004    -2.1928138719
 C1        1.4238055531     1.7115423857    -1.1689072985
 C2        2.2179900560     1.4298878489     1.4483086976
 C3        0.5963967495     1.0388146203    -0.2862416860
 C4        2.6439847882     2.2340655543    -0.7692641334
 C5        3.0334604556     2.0925404637     0.5460040737
 C6        1.0005569035     0.8914388882     1.0389890000
 C7       -0.7330888612     0.4697780703    -0.7281360597
 H3        3.2736304250     2.7431286672    -1.4749213734
 H4        3.9698894617     2.4995482716     0.8837732226
 H6        2.5329351778     1.3454949364     2.4691775887
 C16      -0.6509831458    -0.9437287435    -1.3074353378
 C8       -1.7340820203     0.5620418060     0.4385538909
 N2        0.1831993774     0.1829813818     1.9410863700
 C9       -1.1706573086     0.0149245987     1.7363819785
 C11       0.7293794351    -0.2600616229     3.2236861937
 O1       -1.8961604406    -0.4920974558     2.5579678016
 C18      -0.6272482538    -3.5198607600    -2.3953228780
```

```
  C19      -1.6757406427     -1.3852506179     -2.1286067421
  C20       0.3948170759     -1.8107905017     -1.0533461416
  C21       0.4071169525     -3.0892169264     -1.5911539213
  C22      -1.6725588532     -2.6587689934     -2.6640555997
  H2       -2.4844533180     -0.7232233195     -2.3523000849
  H5        1.2132888071     -1.4923495256     -0.4441174759
  H7        1.2204982509     -3.7472755682     -1.3779370649
  H8       -2.4817072260     -2.9815793727     -3.2883483445
  H9       -0.6208173945     -4.5118840736     -2.8103227851
  H10      -1.1136174370      1.1057319473     -1.5210713933
  C10      -2.2309615982      1.9935644890      0.6785656082
  H11      -1.4186286112      2.6742911328      0.8898375564
  H12      -2.9214182763      2.0170643556      1.5141575279
  H13      -2.7489909940      2.3539788593     -0.2011381038
  H14      -2.5900691670     -0.0656402959      0.2362944114
  H15       1.7087391925     -0.6794418568      3.0764174867
  H16       0.0789870911     -1.0063698160      3.6284353537
  H17       0.7916365960      0.5519518166      3.9354038077

  nuclear repulsion energy.......  1414.177259349 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   4   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.316E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     89     90     89     87     84
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    183    184    195    182    182    185
171
  grid # 4      215    326    327    338    326    326    321
314

  number of gridpoints:
```

```
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     70     92     82     96     81
71
  grid # 2      118    118    111    100     90    104     90
79
  grid # 3      223    223    207    197    174    214    176
142
  grid # 4      224    223    206    340    313    389    297
270

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     86     88     89     89     70
72
  grid # 2      122     97     96     95     97     97    113
112
  grid # 3      261    183    182    182    184    184    213
211
  grid # 4      454    328    326    326    328    328    212
209

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     72     72     71
70
  grid # 2      118    118    118    106     79    109    111
109
  grid # 3      222    222    222    205    152    218    219
216
  grid # 4      223    224    224    199    288    214    219
214

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       68     71     70     71   2861
  grid # 2      109    111    107    109   3726
  grid # 3      211    213    212    217   7182
  grid # 4      206    210    209    215   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
```

	t e r	p d t	i i s	c u t	r i d	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	2	U	-783.00096356699		3.6E-04	2.0E-02
etot	2	Y	Y	6	M	-783.02839546248	2.7E-02	1.8E-04	8.2E-03
etot	3	N	Y	2	U	-783.03220148867	3.8E-03	5.3E-05	2.0E-03
etot	4	Y	Y	6	M	-783.03242887817	2.3E-04	2.2E-05	7.3E-04
etot	5	Y	Y	6	M	-783.03247141414	4.3E-05	7.2E-06	1.9E-04
etot	6	Y	Y	6	M	-783.03247578211	4.4E-06	4.0E-06	5.9E-05
etot	7	Y	N	6	M	-783.03247707189	1.3E-06	0.0E+00	0.0E+00

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.17725934859
   (E)  Total one-electron terms..... -3872.82251182247
   (I)  Total two-electron terms.....  1675.61277540199
   (L)  Electronic energy............. -2197.20973642048  (E+I)
   (N)  Total energy.................  -783.03247707189  (A+L)

 SCFE: SCF energy: HF    -783.03247707189 hartrees   iterations:
7


 HOMO energy:    -0.30343
 LUMO energy:     0.13243

  Orbital energies:
  -20.52554  -15.60269  -11.34683  -11.28722  -11.25507  -11.24863
  -11.24107  -11.24013  -11.23966  -11.23905  -11.23793  -11.23562
  -11.23035  -11.22885  -11.22766  -11.22640  -11.22580  -11.22456
  -11.22231   -1.38939   -1.26900   -1.16701   -1.15058   -1.10859
   -1.03455   -1.02025   -1.01929   -1.01222   -0.96190   -0.93434
   -0.85925   -0.84853   -0.83525   -0.82265   -0.79692   -0.74177
   -0.71127   -0.70241   -0.67046   -0.65052   -0.64838   -0.63655
   -0.63148   -0.61567   -0.61065   -0.60278   -0.59670   -0.58363
   -0.58136   -0.56572   -0.55113   -0.54555   -0.53632   -0.52323
   -0.52072   -0.50782   -0.49768   -0.49655   -0.48575   -0.47028
   -0.46532   -0.42237   -0.40970   -0.34234   -0.33157   -0.32429
   -0.30343    0.13243    0.13469    0.14524    0.15023    0.20529
    0.23251    0.23833    0.24824    0.26118    0.28966

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr
```

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	1.187004E-04	-7.515965E-05	2.063525E-04
2	C1	4.014296E-04	8.481615E-04	-1.460523E-03
3	C2	-7.614403E-04	-1.655459E-04	1.171509E-03
4	C3	6.178823E-04	1.301631E-03	-2.779853E-03
5	C4	-1.456725E-03	6.135702E-05	-3.095792E-03
6	C5	-2.698911E-04	-8.775386E-04	2.298492E-03
7	C6	2.002173E-03	4.890475E-04	1.158658E-03
8	C7	-9.801192E-05	-1.981019E-04	-2.117659E-04
9	H3	1.989689E-04	6.030181E-04	-7.282828E-04
10	H4	1.835565E-04	-1.063414E-06	1.301840E-04
11	H6	1.047992E-04	-1.728119E-04	5.922276E-04
12	C16	1.925531E-03	3.844211E-03	1.666660E-03
13	C8	-4.154271E-04	-2.392776E-03	1.029371E-03
14	N2	-7.082891E-03	-4.535679E-03	9.482218E-03
15	C9	-2.602550E-03	-2.163163E-03	7.533282E-03
16	C11	-3.542308E-03	3.136769E-03	-4.975745E-03
17	O1	1.338142E-02	5.990080E-03	-1.004035E-02
18	C18	1.079159E-03	-3.459922E-03	-4.940240E-04
19	C19	-2.735162E-03	-2.594389E-03	-2.087062E-03
20	C20	3.343149E-03	-3.144038E-03	8.572842E-04
21	C21	-1.315762E-03	2.256393E-03	1.011987E-03
22	C22	-2.614262E-03	1.724963E-03	-7.381189E-04
23	H2	-5.826829E-03	3.511676E-03	-1.710841E-03
24	H5	3.359092E-03	5.321039E-04	2.670099E-03
25	H7	5.580438E-03	-3.052526E-03	1.640127E-03
26	H8	-2.796019E-03	1.579354E-04	-2.238583E-03
27	H9	3.221615E-04	-3.862745E-04	-5.039925E-05
28	H10	-2.254654E-04	2.770558E-04	-4.822937E-04
29	C10	-1.950680E-03	-6.889848E-04	1.301045E-03
30	H11	2.580893E-03	1.722095E-03	4.536402E-04
31	H12	-1.225009E-05	-3.370148E-04	-3.233219E-04
32	H13	-1.100025E-03	8.970211E-04	-1.533985E-03
33	H14	-1.297947E-03	-8.756878E-05	-1.209862E-03
34	H15	4.152684E-03	-1.818351E-03	-1.256293E-03
35	H16	-3.889406E-03	-4.065049E-03	9.489436E-04
36	H17	8.271764E-04	3.214817E-03	9.312493E-04
total		1.861618E-04	3.523792E-04	-3.337671E-04

end of program der1b

start of program geopt 5

geometry optimization step 5

```
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:           3.4374E-05 *  (  5.0000E-05 )
  gradient maximum:        1.7372E-02 .  (  4.5000E-04 )
  gradient rms:            3.0866E-03 .  (  3.0000E-04 )
  step size:   0.16544  trust radius:   0.30000
  displacement maximum:    7.0718E-02 .  (  1.8000E-03 )
  displacement rms:        1.4979E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.1825E-03    geom step:   1.6544E-
01    full step:   1.6544E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.5403E-03     y:    -9.8162E-04     z:    -2.6062E-03

  new geometry:
                                angstroms
  atom           x                 y                 z
  H1        1.0987118325      1.8395543573     -2.1999368286
  C1        1.4141836402      1.7325800786     -1.1747410342
  C2        2.2079474432      1.4464795417      1.4483511136
  C3        0.5887749833      1.0554537280     -0.2923175807
  C4        2.6314949866      2.2594703294     -0.7720332069
  C5        3.0216143057      2.1122077268      0.5448147951
  C6        0.9900706883      0.9105241030      1.0367872361
  C7       -0.7373084835      0.4795189495     -0.7365492130
  H3        3.2593111208      2.7768224263     -1.4760871088
  H4        3.9606445517      2.5173810426      0.8824559192
  H6        2.5270320159      1.3539817038      2.4700544709
  C16      -0.6516175590     -0.9398224740     -1.2982696610
  C8       -1.7407710715      0.5735214205      0.4283994225
  N2        0.1699923855      0.2018941276      1.9461828094
  C9       -1.1678891560     -0.0025522642      1.7109287725
  C11       0.7356281031     -0.3013954804      3.1864086240
  O1       -1.8609468652     -0.5747958028      2.4956096068
  C18      -0.6237789585     -3.5271827454     -2.3529926481
  C19      -1.6685340606     -1.3806005304     -2.1369223149
  C20       0.3873166884     -1.8132248068     -1.0044955855
  C21       0.4005628849     -3.0987065760     -1.5265741655
  C22      -1.6621537848     -2.6602030620     -2.6580089716
  H2       -2.4767337670     -0.7147731826     -2.3856707687
  H5        1.1961101458     -1.4960729267     -0.3721531500
  H7        1.2107563871     -3.7624724501     -1.2840323475
  H8       -2.4638595052     -2.9804163264     -3.3034488262
  H9       -0.6149999484     -4.5249075837     -2.7576672169
  H10      -1.1196782873      1.1084045557     -1.5371345252
  C10      -2.2101879934      2.0135325539      0.6896778270
  H11      -1.3797349218      2.6761724580      0.9143090483
```

```
  H12      -2.9009236513      2.0370252332      1.5248857927
  H13      -2.7199057493      2.4011167001     -0.1872131765
  H14      -2.6129286232     -0.0334959701      0.2124107304
  H15       1.7064801047     -0.7438772974      2.9994467822
  H16       0.0692473637     -1.0479863456      3.5825710501
  H17       0.8406708959      0.4903666620      3.9202055479

  nuclear repulsion energy.......  1415.828065416 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   5   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.353E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     88     90     89     87     84
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    183    184    194    182    182    185
171
  grid # 4      215    326    327    336    326    326    323
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     70     92     82     95     81
69
  grid # 2      118    118    112    100     90    106     91
79
  grid # 3      223    223    207    197    174    210    175
142
  grid # 4      224    223    208    340    311    390    291
272

  number of gridpoints:
```

```
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      260    184    183    182    184    185    213
211
  grid # 4      455    328    326    327    327    328    214
208

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     73     72     71
71
  grid # 2      118    118    118    106     80    109    111
110
  grid # 3      223    223    224    204    149    216    219
217
  grid # 4      223    224    224    203    289    216    220
218

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    111    107    110   3735
  grid # 3      212    213    213    217   7179
  grid # 4      207    211    209    217   9927

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                          RMS     maximum
      t  p  i  c  r                          energy  density   DIIS
      e  d  i  u  i                          change  change    error
      r  t  s  t  d     total energy

etot  1  N  N  2  U  -783.02597400383                    2.1E-04  4.7E-03
etot  2  Y  Y  6  M  -783.03241189408  6.4E-03  8.4E-05  1.6E-03
etot  3  N  Y  2  U  -783.03317956407  7.7E-04  2.0E-05  5.4E-04
etot  4  Y  Y  6  M  -783.03321306549  3.4E-05  9.6E-06  2.0E-04
etot  5  Y  Y  6  M  -783.03322573189  1.3E-05  3.5E-06  8.0E-05
etot  6  Y  N  6  M  -783.03322453549 -1.2E-06  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.82806541582
   (E)  Total one-electron terms..... -3876.16654809424
   (I)  Total two-electron terms.....  1677.30525814292
   (L)  Electronic energy............. -2198.86128995132  (E+I)
   (N)  Total energy.................  -783.03322453549  (A+L)

 SCFE: SCF energy: HF    -783.03322453549 hartrees   iterations:
6


 HOMO energy:    -0.30318
 LUMO energy:     0.13269

  Orbital energies:
 -20.52404  -15.59966  -11.34325  -11.28686  -11.25522  -11.24863
 -11.24140  -11.24052  -11.24005  -11.23944  -11.23924  -11.23602
 -11.23093  -11.23074  -11.22958  -11.22827  -11.22758  -11.22643
 -11.22341   -1.39841   -1.26863   -1.16574   -1.14929   -1.10761
  -1.03275   -1.01896   -1.01851   -1.01154   -0.96033   -0.93303
  -0.85749   -0.84733   -0.83408   -0.82061   -0.79583   -0.74095
  -0.71048   -0.70045   -0.67056   -0.65025   -0.64812   -0.63633
  -0.63120   -0.61502   -0.61154   -0.60123   -0.59687   -0.58347
  -0.58113   -0.56504   -0.54880   -0.54570   -0.53540   -0.52334
  -0.52010   -0.50669   -0.49877   -0.49603   -0.48540   -0.46985
  -0.46502   -0.42074   -0.40834   -0.34176   -0.33211   -0.32274
  -0.30318    0.13269    0.13430    0.14490    0.14931    0.20919
   0.23163    0.23804    0.24590    0.26009    0.28867

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

 atom  label         x             y             z
 ----  -----   -------------  -------------  -------------
   1    H1      1.675721E-04  -1.164981E-04   8.468534E-04
   2    C1      2.002624E-04   4.928235E-04  -8.570723E-04
   3    C2      2.992181E-06   2.277514E-05   5.629316E-04
   4    C3      7.909091E-04   1.123698E-03  -1.029025E-03
   5    C4     -5.666933E-04   2.096215E-04  -1.621562E-03
   6    C5      4.049877E-04  -3.538448E-04   1.688360E-03
```

7	C6	5.872342E-04	-1.002550E-03	3.276145E-03
8	C7	-1.461532E-03	9.125176E-04	-7.554179E-04
9	H3	-3.809159E-04	-2.893079E-04	3.054658E-04
10	H4	-8.549588E-04	-2.638272E-04	-2.289291E-04
11	H6	-6.725574E-04	2.183269E-04	-1.224473E-03
12	C16	3.056431E-03	1.169990E-03	8.876220E-04
13	C8	-3.947226E-04	1.167398E-04	1.808986E-04
14	N2	2.263462E-03	1.732744E-03	-6.111698E-03
15	C9	5.850544E-03	3.034761E-03	-4.917864E-03
16	C11	-1.018353E-03	-4.035924E-04	1.762748E-03
17	O1	-7.557601E-03	-4.659006E-03	6.967255E-03
18	C18	4.277214E-04	-1.544302E-03	-1.333327E-04
19	C19	-2.008165E-03	-4.390206E-04	-8.999623E-04
20	C20	4.159773E-04	-9.812098E-05	7.362616E-04
21	C21	-1.686095E-03	6.848704E-05	-4.396321E-04
22	C22	-8.364665E-04	-1.642458E-03	-1.439833E-03
23	H2	-7.142391E-04	6.971094E-04	-1.776284E-04
24	H5	-2.087682E-04	7.006852E-05	-2.827353E-04
25	H7	6.573289E-04	-2.941138E-04	3.534378E-05
26	H8	1.146995E-03	4.068772E-04	7.106086E-04
27	H9	1.863614E-04	5.931925E-04	2.503962E-04
28	H10	5.139008E-04	-5.307195E-04	5.809641E-04
29	C10	9.233737E-04	7.904455E-04	1.284104E-04
30	H11	-6.205778E-04	-5.189377E-04	-2.777039E-04
31	H12	-2.512100E-04	-8.469830E-05	-2.048055E-04
32	H13	-1.145209E-04	-4.017320E-05	3.362203E-04
33	H14	1.686984E-03	4.567354E-04	5.540596E-04
34	H15	-5.362436E-04	2.281842E-04	-5.004878E-04
35	H16	-4.393583E-05	-2.340951E-04	-5.368865E-05
36	H17	8.398658E-04	3.891635E-04	8.513466E-04
total		1.953463E-04	2.189955E-04	-4.939585E-04

end of program der1b

start of program geopt 6

geometry optimization step 6
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format

energy change: -7.4746E-04 . (5.0000E-05)
gradient maximum: 1.1222E-02 . (4.5000E-04)
gradient rms: 1.3753E-03 . (3.0000E-04)
step size: 0.14346 trust radius: 0.30000
displacement maximum: 7.2326E-02 . (1.8000E-03)

```
  displacement rms:        1.2988E-02 .  (  1.2000E-03 )
  predicted energy change:    -3.4038E-04    geom step:   1.4346E-
01    full step:   1.4346E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.5551E-03     y:     5.5350E-03     z:     1.5789E-03

  new geometry:
                                 angstroms
  atom            x                y                z
  H1         1.0801660630     1.8882146155    -2.1980470207
  C1         1.4043101703     1.7637006482    -1.1790517006
  C2         2.2171358013     1.4281609211     1.4402146704
  C3         0.5920484779     1.0627607658    -0.3016633957
  C4         2.6196246935     2.2901996458    -0.7733533632
  C5         3.0189180121     2.1163892674     0.5418548268
  C6         1.0022372601     0.8929567425     1.0260158942
  C7        -0.7355433925     0.4813585973    -0.7416683094
  H3         3.2389980795     2.8271955913    -1.4701002422
  H4         3.9549877170     2.5226661976     0.8805388361
  H6         2.5408524327     1.3198336843     2.4565391994
  C16       -0.6468414940    -0.9412370247    -1.2998974489
  C8        -1.7326810113     0.5759065138     0.4292181215
  N2         0.1872505976     0.1672359993     1.9213605063
  C9        -1.1612964033     0.0092929335     1.7151904478
  C11        0.7363515604    -0.3331652384     3.1689455392
  O1        -1.8763759804    -0.5111855715     2.5260341186
  C18       -0.6256862983    -3.5426672544    -2.3366816654
  C19       -1.6642925482    -1.3847844507    -2.1500633631
  C20        0.3771278873    -1.8238165705    -0.9827589264
  C21        0.3815805454    -3.1159670229    -1.4925486977
  C22       -1.6533000303    -2.6686454310    -2.6666506642
  H2        -2.4712111135    -0.7157725968    -2.4142554675
  H5         1.1820663271    -1.5100840973    -0.3421502507
  H7         1.1876352664    -3.7830571499    -1.2304751274
  H8        -2.4384418876    -2.9813153157    -3.3300159761
  H9        -0.6118293347    -4.5404666663    -2.7360234260
  H10       -1.1207548192     1.1056422804    -1.5407053179
  C10       -2.2109909388     2.0130706588     0.6859832063
  H11       -1.3865451720     2.6803962402     0.9079369547
  H12       -2.9037995456     2.0323688466     1.5189354328
  H13       -2.7240673484     2.3934890835    -0.1903800121
  H14       -2.5960103008    -0.0386542713     0.2224367318
  H15        1.6958727895    -0.8010305494     2.9784069828
  H16        0.0467660819    -1.0606078772     3.5657880936
  H17        0.8707108077     0.4596959140     3.8982617645

  nuclear repulsion energy.......  1415.066943187 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   6   /
 ------------------------------------------------
```

```
  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.385E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     88     88     89     88     85
81
  grid # 2      116     95     95     98     97     97     93
90
  grid # 3      215    182    182    193    182    183    191
171
  grid # 4      215    326    327    336    326    326    324
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     71     89     82     95     81
68
  grid # 2      118    118    112     98     90    105     91
78
  grid # 3      224    223    207    196    174    212    176
149
  grid # 4      224    223    207    342    312    389    294
275

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     88     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      261    183    183    182    183    185    215
211
  grid # 4      454    328    327    327    327    329    214
208
```

```
  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     73     72     71
71
  grid # 2      118    118    118    106     81    109    110
110
  grid # 3      223    223    224    203    151    218    218
217
  grid # 4      223    223    224    199    287    216    220
219

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       68     71     70     71   2858
  grid # 2      109    109    108    111   3728
  grid # 3      214    214    212    217   7197
  grid # 4      206    212    209    219   9932

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  2  U  -783.02847022184           1.7E-04  3.7E-03
etot   2  Y  Y  6  M  -783.03270652417  4.2E-03  6.9E-05  1.4E-03
etot   3  Y  Y  6  M  -783.03324029720  5.3E-04  1.7E-05  3.6E-04
etot   4  N  Y  2  U  -783.03326918803  2.9E-05  1.0E-05  1.7E-04
etot   5  Y  Y  6  M  -783.03328006917  1.1E-05  4.2E-06  6.2E-05
etot   6  Y  N  6  M  -783.03328503981  5.0E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.06694318720
   (E)  Total one-electron terms..... -3874.62895415063
   (I)  Total two-electron terms.....  1676.52872592362
   (L)  Electronic energy............. -2198.10022822701  (E+I)
   (N)  Total energy.................  -783.03328503981  (A+L)

 SCFE: SCF energy: HF    -783.03328503981 hartrees   iterations:
6
```

```
HOMO energy:    -0.30318
LUMO energy:     0.13205

 Orbital energies:
 -20.52437  -15.60129  -11.34446  -11.28759  -11.25584  -11.24877
 -11.24238  -11.24099  -11.24051  -11.23981  -11.23968  -11.23635
 -11.23164  -11.23121  -11.22995  -11.22978  -11.22762  -11.22697
 -11.22263   -1.39479   -1.27028   -1.16488   -1.14876   -1.10745
  -1.03252   -1.02039   -1.01749   -1.01108   -0.96055   -0.93317
  -0.85794   -0.84823   -0.83401   -0.81995   -0.79588   -0.74214
  -0.71077   -0.70000   -0.67056   -0.65082   -0.64803   -0.63591
  -0.63121   -0.61559   -0.61090   -0.60207   -0.59673   -0.58304
  -0.58035   -0.56470   -0.54963   -0.54513   -0.53528   -0.52345
  -0.51977   -0.50684   -0.49802   -0.49581   -0.48546   -0.46977
  -0.46467   -0.42105   -0.40899   -0.34182   -0.33189   -0.32296
  -0.30318    0.13205    0.13436    0.14392    0.14895    0.20697
   0.23199    0.23810    0.24531    0.26008    0.28885

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H1     -1.795944E-04  -3.118038E-05  -5.583791E-05
  2    C1     -9.321471E-04  -1.054422E-03   1.537852E-03
  3    C2      3.738172E-04   5.618182E-04  -1.604693E-03
  4    C3      4.633339E-04  -4.790657E-04   8.062807E-04
  5    C4      9.243828E-04  -2.522562E-04   2.710321E-03
  6    C5     -9.761166E-04   2.168077E-04  -1.855734E-03
  7    C6     -7.223444E-04   2.808002E-04  -2.805185E-03
  8    C7      1.080853E-03  -2.615386E-04   6.869812E-04
  9    H3     -1.144663E-04  -2.874108E-04   5.832668E-04
 10    H4      4.603399E-04   1.843548E-04   1.776106E-04
 11    H6      2.764464E-04   5.832878E-05   3.241626E-04
 12    C16    -2.695592E-03  -9.096535E-04  -1.068647E-03
 13    C8      1.226026E-03   2.439918E-04  -1.106270E-04
 14    N2     -3.287839E-03   3.994052E-04  -3.612303E-04
 15    C9     -1.059492E-03   1.376003E-03  -5.188573E-04
 16    C11     2.263417E-03  -2.016954E-03   8.502285E-04
 17    O1      2.165463E-03  -2.488891E-04  -5.789309E-04
```

18	C18	-1.253331E-03	8.327719E-04	-1.439723E-04
19	C19	1.543027E-03	6.599472E-04	6.523318E-04
20	C20	-4.201192E-04	3.846237E-04	1.701998E-04
21	C21	2.997552E-03	-1.857672E-04	8.678890E-04
22	C22	1.367939E-03	1.530209E-03	1.016037E-03
23	H2	2.246596E-03	-1.181870E-03	6.893478E-04
24	H5	-9.109077E-04	-2.534294E-04	-7.596963E-04
25	H7	-1.535738E-03	8.203099E-04	-5.485205E-04
26	H8	-1.046588E-03	-8.283496E-04	-4.464758E-04
27	H9	-1.997463E-04	-6.373413E-04	-3.318743E-04
28	H10	-3.080920E-04	4.572585E-04	-6.527283E-04
29	C10	-4.130920E-04	-4.711066E-04	3.445992E-05
30	H11	5.597385E-04	4.950323E-04	1.682091E-04
31	H12	-4.445192E-05	-5.587836E-06	3.099748E-04
32	H13	-3.350458E-04	3.825576E-04	-6.762836E-04
33	H14	-1.590544E-03	-6.651085E-04	-7.114774E-04
34	H15	-9.276383E-04	-6.500667E-05	6.632606E-04
35	H16	1.566907E-03	8.756548E-04	2.830984E-04
36	H17	-4.744247E-04	1.974400E-04	1.036124E-04
---		---	---	---
total		8.852801E-05	1.223778E-04	-5.956472E-04

```
 end of program der1b


 start of program geopt   7

 geometry optimization step  7
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:          -6.0504E-05 .  (  5.0000E-05 )
 gradient maximum:        4.4434E-03 .  (  4.5000E-04 )
 gradient rms:            1.1093E-03 .  (  3.0000E-04 )
 step size:   0.06659  trust radius:   0.30000
 displacement maximum:    2.9978E-02 .  (  1.8000E-03 )
 displacement rms:        6.0288E-03 .  (  1.2000E-03 )
 predicted energy change:    -1.8030E-04    geom step:   6.6590E-
02    full step:   6.6590E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -8.2632E-05     y:    -3.2548E-03     z:    -8.9091E-04

 new geometry:
                              angstroms
 atom            x                y                z
```

```
 H1        1.0923157777      1.8511908883     -2.1983526231
 C1        1.4115167194      1.7404583347     -1.1764782013
 C2        2.2099688298      1.4438968105      1.4446995987
 C3        0.5918972532      1.0559313783     -0.2957570059
 C4        2.6268091160      2.2688179827     -0.7727834141
 C5        3.0184723991      2.1172746070      0.5434999002
 C6        0.9967751625      0.9023081325      1.0324585438
 C7       -0.7361843676      0.4789582401     -0.7372607371
 H3        3.2521285827      2.7905806029     -1.4739093469
 H4        3.9537253111      2.5274064273      0.8821154777
 H6        2.5278775393      1.3520470460      2.4643436594
 C16      -0.6491288396     -0.9400839860     -1.3020108980
 C8       -1.7351623108      0.5694397388      0.4321267872
 N2        0.1811873010      0.1843246012      1.9335737921
 C9       -1.1606918280      0.0033139557      1.7170309233
 C11       0.7416417813     -0.3064363905      3.1853941553
 O1       -1.8647412193     -0.5393972714      2.5222979362
 C18      -0.6296562981     -3.5337966928     -2.3543800013
 C19      -1.6621038763     -1.3773739128     -2.1546452184
 C20       0.3741754249     -1.8236368726     -0.9917479192
 C21       0.3833296702     -3.1102979459     -1.5123563264
 C22      -1.6564765951     -2.6585532519     -2.6763622249
 H2       -2.4625438045     -0.7045477710     -2.4144940478
 H5        1.1754945077     -1.5138870138     -0.3491529199
 H7        1.1894433583     -3.7786656821     -1.2587161724
 H8       -2.4479794746     -2.9716827610     -3.3351256950
 H9       -0.6188686438     -4.5305264830     -2.7591191323
 H10      -1.1199373585      1.1086564633     -1.5348986584
 C10      -2.2153192858      2.0058706778      0.6907562246
 H11      -1.3904688093      2.6746020953      0.9120554439
 H12      -2.9065154333      2.0238184668      1.5258496381
 H13      -2.7313156619      2.3880483454     -0.1846431288
 H14      -2.5999536632     -0.0459889345      0.2211875259
 H15       1.6981688916     -0.7729477461      2.9942200459
 H16       0.0643131306     -1.0332821968      3.5993257589
 H17       0.8743537234      0.4942438937      3.9054017493

 nuclear repulsion energy.......  1415.254391435 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   7   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.340E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
```

```
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     89     88     89     87     84
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    182    183    195    182    182    192
171
  grid # 4      215    326    327    336    326    326    324
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     70     90     82     95     81
70
  grid # 2      118    118    112    100     90    104     90
79
  grid # 3      224    223    207    196    174    212    176
141
  grid # 4      224    223    207    342    313    389    293
272

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      261    184    183    182    184    185    214
211
  grid # 4      455    328    326    327    327    328    214
208

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     72     72     71
71
  grid # 2      118    118    118    106     79    109    111
110
  grid # 3      223    223    224    203    152    218    219
217
  grid # 4      223    224    224    199    288    216    220
219
```

```
  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2860
  grid # 2      110    111    108    111   3733
  grid # 3      214    214    212    217   7195
  grid # 4      207    211    209    217   9928

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03211337809           9.1E-05  2.1E-03
etot   2  Y  Y  4  M  -783.03315263951  1.0E-03  3.5E-05  8.2E-04
etot   3  Y  Y  4  M  -783.03328396338  1.3E-04  9.4E-06  2.0E-04
etot   4  Y  Y  4  M  -783.03329030749  6.3E-06  5.0E-06  9.5E-05
etot   5  Y  N  4  M  -783.03329301658  2.7E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1415.25439143469
   (E)  Total one-electron terms..... -3875.00899226867
   (I)  Total two-electron terms.....  1676.72130781740
   (L)  Electronic energy..... -2198.28768445127  (E+I)
   (N)  Total energy.............  -783.03329301658  (A+L)

 SCFE: SCF energy: HF    -783.03329301658 hartrees   iterations:
5


 HOMO energy:    -0.30336
 LUMO energy:     0.13266

  Orbital energies:
  -20.52329  -15.60116  -11.34402  -11.28707  -11.25578  -11.24896
  -11.24176  -11.24038  -11.24016  -11.23972  -11.23905  -11.23569
  -11.23088  -11.23074  -11.22977  -11.22899  -11.22755  -11.22634
  -11.22317   -1.39451   -1.26957   -1.16549   -1.14939   -1.10770
   -1.03300   -1.01983   -1.01809   -1.01147   -0.96121   -0.93326
   -0.85792   -0.84826   -0.83447   -0.82060   -0.79599   -0.74184
   -0.71088   -0.70037   -0.67046   -0.65055   -0.64828   -0.63600
   -0.63140   -0.61543   -0.61084   -0.60172   -0.59652   -0.58328
```

```
 -0.58063   -0.56492   -0.54948   -0.54499   -0.53546   -0.52329
 -0.52040   -0.50711   -0.49811   -0.49608   -0.48509   -0.47001
 -0.46487   -0.42106   -0.40862   -0.34209   -0.33185   -0.32295
 -0.30336    0.13266    0.13428    0.14423    0.14938    0.20781
  0.23187    0.23796    0.24562    0.25997    0.28874

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -2.561799E-05   1.441824E-04  -3.469907E-04
  2    C1     -2.375602E-04  -5.189115E-05   4.973580E-05
  3    C2     -1.370691E-04  -1.393459E-04   2.721944E-04
  4    C3     -2.001109E-04  -1.003181E-04  -1.659379E-04
  5    C4      2.766633E-05   1.440521E-04  -4.446108E-04
  6    C5      2.841382E-04   1.425504E-04   4.197984E-04
  7    C6      5.871213E-05  -1.389429E-04  -2.994472E-04
  8    C7      3.169600E-04   1.369830E-04  -1.683716E-04
  9    H3      1.444461E-04   2.789461E-04  -2.913196E-04
 10    H4     -3.651574E-05  -3.589678E-05   6.358694E-06
 11    H6      1.599072E-04  -2.060178E-04   4.183373E-04
 12    C16    -1.405498E-03  -1.395263E-04  -7.016079E-04
 13    C8     -1.158821E-04  -1.535882E-04  -2.565339E-04
 14    N2      6.855257E-04   8.506849E-05   9.384433E-04
 15    C9     -1.021740E-03  -2.752968E-04   7.982523E-04
 16    C11    -7.002099E-04  -1.501068E-04  -5.353494E-04
 17    O1     -8.791091E-05  -5.193848E-05  -4.944080E-04
 18    C18     7.113236E-04  -1.871434E-04   2.746115E-04
 19    C19     2.913371E-04   5.497427E-05   2.558909E-06
 20    C20     3.289849E-04  -4.423926E-04   3.414301E-05
 21    C21     4.384409E-04  -1.017656E-03  -1.159728E-04
 22    C22    -2.656651E-04   6.004971E-04  -1.353645E-05
 23    H2     -9.054830E-05   2.214191E-05  -1.142243E-04
 24    H5      8.232658E-04   2.969922E-04   4.361003E-04
 25    H7     -8.304240E-04   5.272169E-04  -1.672065E-04
 26    H8      1.221024E-04   6.833266E-05   1.548769E-04
 27    H9     -5.034033E-06  -1.803031E-06   2.562835E-05
 28    H10     3.541751E-05  -1.991384E-04   1.358901E-04
 29    C10    -3.949816E-04   3.532173E-04   4.657291E-05
```

```
  30    H11    -1.416711E-05   6.119304E-05   1.550520E-05
  31    H12     1.775882E-04   2.823262E-05  -4.585842E-05
  32    H13     1.021600E-04  -7.351969E-05  -1.879154E-05
  33    H14     5.194675E-05   8.506471E-05   3.261954E-06
  34    H15     1.187325E-03  -2.931321E-04  -5.627831E-05
  35    H16    -3.344376E-04   2.565469E-04  -3.995527E-04
  36    H17     2.653277E-05   4.990028E-04   1.562437E-04
 -----------   -------------  -------------  -------------
   total       7.040787E-05   1.275403E-04  -4.474850E-04

  end of program der1b


  start of program geopt   8

  geometry optimization step  8
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -7.9768E-06 *  (  5.0000E-05 )
  gradient maximum:        1.2001E-03 .  (  4.5000E-04 )
  gradient rms:            3.6847E-04 .  (  3.0000E-04 )
  step size:   0.05347  trust radius:   0.30000
  displacement maximum:    1.6820E-02 .  (  1.8000E-03 )
  displacement rms:        4.8410E-03 .  (  1.2000E-03 )
  predicted energy change:    -4.9411E-05    geom step:   5.3471E-
02    full step:   5.3471E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.4793E-03     y:    -1.5748E-03     z:    -1.5199E-03

  new geometry:
                                angstroms
  atom            x                y                z
  H1        1.0816861330     1.8840425267    -2.1951883136
  C1        1.4041030358     1.7605003712    -1.1745775370
  C2        2.2120903169     1.4328644204     1.4412821016
  C3        0.5896380418     1.0612002718    -0.2991853718
  C4        2.6186438265     2.2899591325    -0.7685117424
  C5        3.0161554441     2.1204797745     0.5447527791
  C6        0.9970350021     0.8966147796     1.0269105617
  C7       -0.7362568597     0.4817290556    -0.7421179592
  H3        3.2383096475     2.8265772164    -1.4655445753
  H4        3.9523879644     2.5275136102     0.8849854941
  H6        2.5356115176     1.3260669481     2.4591629655
  C16      -0.6487457754    -0.9408717006    -1.2994812195
  C8       -1.7362167606     0.5790049353     0.4266407924
  N2        0.1800676838     0.1774452016     1.9276499701
```

```
  C9       -1.1650752636      0.0005935379      1.7091490781
  C11       0.7404984501     -0.3241058656      3.1724009862
  O1       -1.8707435440     -0.5495828139      2.5065623157
  C18      -0.6263613548     -3.5404913230     -2.3356614436
  C19      -1.6580973795     -1.3827123619     -2.1506745151
  C20       0.3781896041     -1.8210878297     -0.9842938338
  C21       0.3866546999     -3.1119249236     -1.4959993720
  C22      -1.6524333150     -2.6669533162     -2.6636735813
  H2       -2.4570889226     -0.7123831469     -2.4158833258
  H5        1.1822529226     -1.5042674077     -0.3440280414
  H7        1.1853170011     -3.7796722047     -1.2351522628
  H8       -2.4452078201     -2.9863119135     -3.3200572095
  H9       -0.6191429954     -4.5407029991     -2.7330776765
  H10      -1.1202192645      1.1063861556     -1.5430642266
  C10      -2.2030352195      2.0205614600      0.6910274193
  H11      -1.3710122931      2.6817364715      0.9134320485
  H12      -2.8911418488      2.0425983205      1.5281560251
  H13      -2.7164082476      2.4097011918     -0.1829463897
  H14      -2.6077724674     -0.0267166542      0.2132818415
  H15       1.7034039498     -0.7823660909      2.9817088235
  H16       0.0626279120     -1.0561919523      3.5750172237
  H17       0.8650150069      0.4708523322      3.9000971693

  nuclear repulsion energy.......  1415.538815491 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   8   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.358E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     88     89     89     87     83
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    182    183    195    181    183    189
171
```

```
  grid # 4      215    326    327    336    326    326    324
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     71     91     82     95     81
69
  grid # 2      118    118    112    100     90    105     90
80
  grid # 3      223    223    207    197    174    212    176
143
  grid # 4      224    223    207    340    313    389    293
272

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      261    184    183    182    184    185    215
211
  grid # 4      455    328    326    327    327    328    214
208

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     74     72     71
71
  grid # 2      118    118    118    107     80    109    111
110
  grid # 3      222    223    224    204    147    216    219
217
  grid # 4      223    224    224    199    287    216    220
219

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2862
  grid # 2      110    110    107    111   3735
  grid # 3      214    213    213    217   7188
  grid # 4      207    211    209    217   9925

  end of program grid


  start of program rwr
  end of program rwr
```

```
  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  1  U  -783.03262608496           7.0E-05  1.8E-03
etot  2  Y  Y  4  M  -783.03318790467  5.6E-04  2.6E-05  6.9E-04
etot  3  Y  Y  4  M  -783.03326242701  7.5E-05  7.0E-06  1.6E-04
etot  4  Y  Y  4  M  -783.03326768614  5.3E-06  3.3E-06  6.4E-05
etot  5  Y  N  4  M  -783.03326728739 -4.0E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.53881549128
   (E)  Total one-electron terms..... -3875.58413882566
   (I)  Total two-electron terms.....  1677.01205604700
   (L)  Electronic energy............. -2198.57208277867  (E+I)
   (N)  Total energy.................  -783.03326728739  (A+L)

 SCFE: SCF energy: HF    -783.03326728739 hartrees   iterations:
5


 HOMO energy:    -0.30335
 LUMO energy:     0.13251

  Orbital energies:
  -20.52422  -15.60084  -11.34433  -11.28710  -11.25572  -11.24887
  -11.24187  -11.24060  -11.24017  -11.24002  -11.23942  -11.23611
  -11.23121  -11.23083  -11.22944  -11.22863  -11.22755  -11.22673
  -11.22337   -1.39506   -1.26930   -1.16532   -1.14916   -1.10737
   -1.03244   -1.01967   -1.01820   -1.01119   -0.96068   -0.93312
   -0.85763   -0.84770   -0.83424   -0.82064   -0.79584   -0.74144
   -0.71058   -0.70035   -0.67036   -0.65035   -0.64806   -0.63599
   -0.63133   -0.61524   -0.61098   -0.60158   -0.59670   -0.58304
   -0.58072   -0.56476   -0.54949   -0.54513   -0.53548   -0.52346
   -0.52002   -0.50669   -0.49837   -0.49594   -0.48526   -0.46990
   -0.46480   -0.42088   -0.40862   -0.34176   -0.33181   -0.32300
   -0.30335    0.13251    0.13442    0.14423    0.14927    0.20781
    0.23176    0.23795    0.24555    0.25996    0.28880

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
```

```
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	5.924487E-05	-1.698414E-04	4.945989E-04
2	C1	-4.306166E-04	-1.906763E-04	-2.445113E-04
3	C2	6.945001E-04	4.208680E-04	-5.881157E-05
4	C3	4.153490E-04	2.717039E-04	-8.090204E-04
5	C4	1.220850E-04	1.364500E-04	3.652957E-06
6	C5	-1.960677E-04	-3.286759E-04	4.851748E-04
7	C6	-7.041621E-05	1.367634E-04	9.398904E-04
8	C7	-4.660474E-04	2.548686E-04	1.067902E-04
9	H3	-3.315313E-04	-3.971046E-04	4.474358E-04
10	H4	-1.966963E-04	-6.220120E-05	-3.438675E-06
11	H6	-2.350673E-04	2.210331E-04	-5.897978E-04
12	C16	1.351508E-03	2.531776E-04	4.480387E-04
13	C8	-1.630797E-05	6.884564E-05	2.688462E-04
14	N2	-1.020637E-03	2.139831E-04	-2.159239E-03
15	C9	1.019885E-03	2.978178E-04	-6.807836E-04
16	C11	2.130489E-04	-5.359970E-05	3.094795E-04
17	O1	-1.071569E-04	-2.153301E-04	6.284247E-04
18	C18	7.268573E-05	-2.430718E-04	1.851506E-04
19	C19	-4.091382E-04	-4.544223E-04	-2.505725E-04
20	C20	5.607001E-04	-1.083909E-04	5.326203E-04
21	C21	-1.795300E-03	1.190627E-03	-3.540111E-04
22	C22	-8.173410E-04	-5.378115E-04	-9.088058E-04
23	H2	-8.911332E-04	6.189957E-04	-2.764273E-04
24	H5	-8.524622E-04	-5.050876E-04	-7.049149E-04
25	H7	1.870322E-03	-1.108338E-03	4.169543E-04
26	H8	8.472170E-04	5.514282E-04	6.407214E-04
27	H9	2.861665E-04	3.072477E-04	2.601660E-04
28	H10	9.951616E-05	9.931045E-05	-8.752772E-05
29	C10	8.986294E-04	2.271535E-05	-1.644992E-04
30	H11	-5.936936E-04	-4.761906E-04	-2.246065E-04
31	H12	-2.043974E-04	-7.395980E-05	-5.741068E-05
32	H13	4.280655E-05	-3.540085E-05	1.777502E-04
33	H14	3.718017E-04	1.021524E-04	1.199468E-04
34	H15	-5.126754E-04	-7.471762E-05	-3.759131E-05
35	H16	1.790997E-06	-3.854786E-04	1.042483E-04
36	H17	2.644802E-04	3.809759E-04	5.626473E-04
total		4.505239E-05	1.286655E-04	-4.794324E-04

```
 end of program der1b


 start of program geopt   9
```

```
  geometry optimization step  9
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:           2.5729E-05 *  (  5.0000E-05 )
  gradient maximum:        2.1723E-03 .  (  4.5000E-04 )
  gradient rms:            4.7051E-04 .  (  3.0000E-04 )
  step size:   0.03081  trust radius:   0.30000
  displacement maximum:    1.1611E-02 .  (  1.8000E-03 )
  displacement rms:        2.7898E-03 .  (  1.2000E-03 )
  predicted energy change:    -3.8840E-05    geom step:   3.0814E-
02    full step:   3.0814E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     9.2336E-04     y:     5.5039E-04     z:     4.5133E-04

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1         1.0844844141      1.8701898015     -2.1974597564
  C1         1.4061457753      1.7519299507     -1.1766171090
  C2         2.2124039603      1.4370758334      1.4417698691
  C3         0.5902078799      1.0591653320     -0.2984905716
  C4         2.6215931983      2.2805272972     -0.7717881018
  C5         3.0178554775      2.1180369052      0.5427310546
  C6         0.9974410821      0.8995193672      1.0286405571
  C7        -0.7370767256      0.4808286999     -0.7393413455
  H3         3.2432607067      2.8105750610     -1.4707527196
  H4         3.9541898259      2.5253402884      0.8815668951
  H6         2.5344910545      1.3358407023      2.4599769264
  C16       -0.6500012096     -0.9402810133     -1.3001162044
  C8        -1.7356927734      0.5738069846      0.4303665957
  N2         0.1817746829      0.1803027199      1.9292482414
  C9        -1.1620016596      0.0012289040      1.7133102276
  C11        0.7425555462     -0.3136064032      3.1783946283
  O1        -1.8654660106     -0.5468244684      2.5143123412
  C18       -0.6276428155     -3.5362655489     -2.3442554611
  C19       -1.6591207244     -1.3777797940     -2.1561634447
  C20        0.3727474924     -1.8240405886     -0.9823149942
  C21        0.3813118422     -3.1128753933     -1.4982354250
  C22       -1.6513616476     -2.6599672614     -2.6741729910
  H2        -2.4590212935     -0.7053173881     -2.4214471080
  H5         1.1727008484     -1.5127940672     -0.3372649560
  H7         1.1824177497     -3.7822724134     -1.2375707695
  H8        -2.4388510614     -2.9732227544     -3.3363716591
```

```
  H9       -0.6169260698     -4.5342742140     -2.7456222569
  H10      -1.1214724801      1.1078460911     -1.5383312899
  C10      -2.2101790577      2.0118794381      0.6926020483
  H11      -1.3832236519      2.6773280821      0.9147759230
  H12      -2.8998683380      2.0306429003      1.5286602273
  H13      -2.7250692209      2.3972836550     -0.1817385072
  H14      -2.6032404246     -0.0371573901      0.2187239683
  H15       1.7029194243     -0.7778244670      2.9890138378
  H16       0.0631335767     -1.0416626789      3.5870589328
  H17       0.8717192541      0.4864178078      3.9014030282

  nuclear repulsion energy.......  1415.473951373 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   9   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.353E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     88     88     89     87     84
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    182    183    195    181    183    192
171
  grid # 4      215    326    327    336    326    326    324
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     71     90     82     95     81
70
  grid # 2      118    118    112    100     90    105     90
80
  grid # 3      223    223    207    198    174    212    176
143
```

```
  grid # 4      224    223    207    342    312    390    293
273

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      261    184    183    182    184    185    215
211
  grid # 4      455    328    326    327    327    328    214
208

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     71     72     71
71
  grid # 2      118    118    118    105     79    109    111
110
  grid # 3      222    223    224    202    156    216    218
217
  grid # 4      223    223    224    199    290    216    220
219

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2859
  grid # 2      110    111    108    111   3734
  grid # 3      214    213    212    217   7197
  grid # 4      207    211    209    218   9931

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                          RMS    maximum
      t  p  i  c  r                                 energy density   DIIS
      e  d  i  u  i                  total energy   change change    error

etot  1  N  N  1  U  -783.03311925796                      4.7E-05  9.5E-04
etot  2  Y  Y  4  M  -783.03329464641  1.8E-04  1.5E-05  3.7E-04
etot  3  Y  Y  4  M  -783.03331774901  2.3E-05  3.9E-06  9.8E-05
etot  4  Y  N  4  M  -783.03331961579  1.9E-06  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1415.47395137304
   (E)  Total one-electron terms..... -3875.45222845079
   (I)  Total two-electron terms.....  1676.94495746196
   (L)  Electronic energy..... -2198.50727098884  (E+I)
   (N)  Total energy.............  -783.03331961579  (A+L)

 SCFE: SCF energy: HF    -783.03331961579 hartrees   iterations:
4


 HOMO energy:    -0.30318
 LUMO energy:     0.13261

  Orbital energies:
 -20.52389  -15.60093  -11.34409  -11.28711  -11.25606  -11.24885
 -11.24177  -11.24028  -11.24025  -11.23993  -11.23919  -11.23587
 -11.23101  -11.23068  -11.22966  -11.22909  -11.22745  -11.22649
 -11.22306   -1.39506   -1.26950   -1.16531   -1.14918   -1.10756
  -1.03275   -1.01967   -1.01809   -1.01135   -0.96076   -0.93322
  -0.85780   -0.84803   -0.83432   -0.82042   -0.79597   -0.74168
  -0.71071   -0.70034   -0.67046   -0.65042   -0.64806   -0.63596
  -0.63140   -0.61535   -0.61093   -0.60157   -0.59668   -0.58325
  -0.58073   -0.56482   -0.54931   -0.54506   -0.53544   -0.52342
  -0.52017   -0.50684   -0.49829   -0.49604   -0.48527   -0.46995
  -0.46477   -0.42097   -0.40867   -0.34193   -0.33192   -0.32291
  -0.30318    0.13261    0.13443    0.14416    0.14933    0.20787
   0.23206    0.23808    0.24564    0.26000    0.28882

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1      2.653930E-05   1.283737E-05   5.879594E-05
   2    C1      3.465086E-05   3.977592E-05   5.907003E-05
   3    C2      4.118131E-05   1.260658E-05  -3.790428E-05
   4    C3      1.139528E-04   7.019300E-05  -2.649424E-06
```

5	C4	-5.053707E-05	-3.462465E-05	7.508451E-05
6	C5	-1.032984E-04	-7.379808E-06	-6.261655E-05
7	C6	1.479133E-05	1.033791E-07	6.770898E-05
8	C7	1.479659E-05	-4.543684E-05	1.438173E-05
9	H3	-1.749304E-05	1.474057E-05	2.759666E-05
10	H4	-1.860931E-05	3.528595E-05	-1.129441E-05
11	H6	-7.209243E-05	2.565000E-05	-1.338413E-04
12	C16	-4.249178E-05	9.263117E-05	-9.882289E-05
13	C8	5.583022E-05	4.732389E-05	3.422178E-05
14	N2	1.341274E-04	1.820265E-04	-1.673886E-04
15	C9	4.217725E-04	5.870173E-05	-4.655713E-04
16	C11	5.083554E-05	-1.141339E-04	2.594866E-04
17	O1	-4.711598E-04	-2.946450E-04	4.512547E-04
18	C18	-4.049014E-05	-9.831823E-05	-4.407278E-05
19	C19	-1.913841E-05	3.446178E-04	7.019929E-05
20	C20	-3.456621E-04	-1.559184E-04	-1.489936E-04
21	C21	1.522859E-04	1.719323E-04	1.368587E-04
22	C22	1.511631E-04	8.144872E-06	-9.173436E-06
23	H2	4.041633E-04	-2.295359E-04	4.489057E-05
24	H5	2.393986E-04	1.277236E-04	2.696163E-05
25	H7	6.796874E-05	-2.422476E-05	1.935922E-06
26	H8	-3.518606E-04	-2.264490E-04	-1.718998E-04
27	H9	-4.573771E-05	-4.964521E-05	-2.099991E-05
28	H10	-2.019072E-05	-8.248216E-06	-2.676481E-05
29	C10	-1.072579E-04	6.001060E-05	-4.385796E-06
30	H11	1.555043E-04	8.839612E-05	-3.058923E-06
31	H12	-5.009177E-05	-8.249944E-06	-2.862638E-05
32	H13	-2.629242E-05	2.779693E-05	-6.925027E-05
33	H14	-3.052893E-05	-5.531269E-05	-4.222350E-05
34	H15	-3.808533E-04	1.568089E-04	-6.691163E-07
35	H16	1.655158E-04	7.330286E-05	-5.891178E-05
36	H17	3.202979E-05	-1.567197E-04	-1.557730E-04
total		8.272150E-05	1.417678E-04	-4.364448E-04

```
 end of program der1b


 start of program geopt  10

 geometry optimization step 10
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:          -5.2328E-05 .  (  5.0000E-05 )
 gradient maximum:        7.2298E-04 .  (  4.5000E-04 )
 gradient rms:            1.4823E-04 *  (  3.0000E-04 )
 step size:   0.01985  trust radius:   0.30000
 displacement maximum:    9.2557E-03 .  (  1.8000E-03 )
```

```
  displacement rms:        1.7968E-03 .  (  1.2000E-03 )
  predicted energy change:    -9.6662E-06    geom step:   1.9847E-
02    full step:   1.9847E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -3.4160E-04     y:     4.3380E-04     z:    -1.0661E-04

  new geometry:
                              angstroms
  atom            x                y                z
  H1        1.0879801414     1.8748513079    -2.1961717168
  C1        1.4082030221     1.7557955777    -1.1751925975
  C2        2.2104278303     1.4394263360     1.4443413822
  C3        0.5921048153     1.0605115239    -0.2992184543
  C4        2.6217774218     2.2861160029    -0.7676712220
  C5        3.0159537020     2.1230325160     0.5473444336
  C6        0.9973706610     0.8998875884     1.0286097720
  C7       -0.7344350112     0.4814952331    -0.7420550785
  H3        3.2436853967     2.8182825519    -1.4648307209
  H4        3.9507179297     2.5324631048     0.8881907809
  H6        2.5304324666     1.3381929042     2.4628679879
  C16      -0.6476150932    -0.9403475856    -1.3010522351
  C8       -1.7341144329     0.5760768822     0.4267143926
  N2        0.1808085506     0.1786588420     1.9267636810

  C9       -1.1623333515     0.0005960869     1.7092261203
  C11       0.7398902540    -0.3220890665     3.1738583173
  O1       -1.8679197186    -0.5471333006     2.5094719797
  C18      -0.6310797670    -3.5405690019    -2.3376143029
  C19      -1.6616671344    -1.3820891979    -2.1495487380
  C20       0.3776631218    -1.8218359150    -0.9881094553
  C21       0.3843249178    -3.1121488437    -1.5005098545
  C22      -1.6583692944    -2.6669556475    -2.6630526898
  H2       -2.4623405509    -0.7113794691    -2.4121537185
  H5        1.1829250301    -1.5069748728    -0.3501791669
  H7        1.1908264693    -3.7785068140    -1.2448539860
  H8       -2.4523531677    -2.9847977060    -3.3175539074
  H9       -0.6228438969    -4.5401318039    -2.7357367734
  H10      -1.1177981737     1.1073708636    -1.5423745734
  C10      -2.2050250193     2.0154024256     0.6896001507
  H11      -1.3765270547     2.6775949378     0.9167962567
  H12      -2.8986113227     2.0342419573     1.5223679953
  H13      -2.7151360787     2.4047262043    -0.1860534962
  H14      -2.6029179885    -0.0327873938     0.2139466596
  H15       1.6978274364    -0.7869965137     2.9815736298
  H16       0.0599281311    -1.0514720881     3.5782560267
  H17       0.8718859681     0.4728282894     3.9005347499

  nuclear repulsion energy.......  1415.527495173 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  10   /
```

```
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.352E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     88     88     89     88     84
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    182    183    194    181    183    194
171
  grid # 4      215    326    327    336    326    326    325
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     71     90     82     95     81
70
  grid # 2      118    118    112    100     90    104     90
80
  grid # 3      223    223    207    196    174    212    176
143
  grid # 4      224    223    207    342    312    390    293
272

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      261    184    183    182    184    185    214
211
  grid # 4      455    328    326    327    327    328    214
208
```

```
  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     71     72     71
71
  grid # 2      118    118    118    106     79    109    111
110
  grid # 3      223    223    224    203    154    216    218
217
  grid # 4      223    224    224    199    290    216    220
219

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2860
  grid # 2      110    110    108    111   3733
  grid # 3      214    213    212    217   7195
  grid # 4      207    211    209    217   9931

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

        i  u  d  i  g                                          RMS    maximum
        t  p  i  c  r                              energy  density   DIIS
        e  d  i  u  i                 total energy change  change    error

etot    1  N  N  1  U  -783.03312256433          2.8E-05  1.5E-03
etot    2  Y  Y  4  M  -783.03327027113  1.5E-04  1.3E-05  5.8E-04
etot    3  Y  Y  4  M  -783.03329103969  2.1E-05  3.9E-06  1.5E-04
etot    4  Y  N  4  M  -783.03329273161  1.7E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1415.52749517283
   (E)  Total one-electron terms..... -3875.56290036481
   (I)  Total two-electron terms.....  1677.00211246037
   (L)  Electronic energy..... -2198.56078790444  (E+I)
   (N)  Total energy.............  -783.03329273161  (A+L)

 SCFE: SCF energy: HF    -783.03329273161 hartrees   iterations:
4


 HOMO energy:    -0.30328
```

```
LUMO energy:     0.13260

 Orbital energies:
 -20.52382  -15.60085  -11.34405  -11.28708  -11.25559  -11.24869
 -11.24177  -11.24025  -11.24011  -11.23985  -11.23920  -11.23596
 -11.23111  -11.23110  -11.22993  -11.22890  -11.22783  -11.22650
 -11.22314   -1.39465   -1.26949   -1.16523   -1.14919   -1.10750
  -1.03267   -1.01982   -1.01796   -1.01126   -0.96091   -0.93318
  -0.85777   -0.84806   -0.83428   -0.82046   -0.79585   -0.74170
  -0.71071   -0.70020   -0.67038   -0.65048   -0.64812   -0.63592
  -0.63120   -0.61540   -0.61085   -0.60162   -0.59653   -0.58309
  -0.58065   -0.56484   -0.54949   -0.54501   -0.53537   -0.52339
  -0.52017   -0.50685   -0.49824   -0.49592   -0.48510   -0.46987
  -0.46476   -0.42092   -0.40859   -0.34194   -0.33178   -0.32295
  -0.30328    0.13260    0.13432    0.14416    0.14929    0.20787
   0.23189    0.23798    0.24548    0.25996    0.28872

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -1.941825E-05   3.282219E-06  -9.680148E-05
  2    C1     -8.285092E-05  -5.758294E-05   1.460040E-04
  3    C2     -1.277475E-05   4.401592E-05  -1.925821E-04
  4    C3      1.395649E-05  -4.789267E-05   1.002244E-05
  5    C4      1.358876E-04   2.394076E-05   1.411143E-04
  6    C5     -6.660862E-06   4.130039E-05  -1.382348E-05
  7    C6     -4.454758E-05  -3.629426E-06  -1.633994E-04
  8    C7      5.509459E-05   6.319051E-05  -1.119585E-05
  9    H3     -2.159103E-05  -2.933819E-05   2.936150E-05
 10    H4     -7.877299E-05  -4.204302E-05  -1.872561E-05
 11    H6      1.085471E-05  -2.641420E-05   1.207225E-04
 12    C16    -6.476354E-04   3.148895E-06  -3.226857E-04
 13    C8      2.007561E-06  -1.247796E-05  -1.196124E-04
 14    N2      4.908766E-05   6.878861E-05  -3.375876E-05
 15    C9     -5.827178E-04   7.181289E-05   1.458682E-04
 16    C11    -1.015523E-04  -1.662537E-04  -1.997109E-04
 17    O1      1.854191E-04   2.418241E-05  -2.865093E-04
 18    C18     4.474830E-04  -4.196247E-05   3.216162E-04
```

```
 19    C19     1.522753E-04  -5.294488E-04  -6.617669E-05
 20    C20     6.154466E-04  -3.835060E-04   2.430588E-04
 21    C21     2.712715E-04  -4.611444E-04  -2.279373E-04
 22    C22    -7.356050E-05   3.923953E-04  -5.230400E-05
 23    H2     -3.236928E-04   3.462680E-04  -1.237701E-04
 24    H5     -2.275290E-04  -1.409874E-04  -1.953462E-04
 25    H7     -6.294574E-04   2.604380E-04  -1.173832E-04
 26    H8      5.272549E-04   3.251973E-04   3.826196E-04
 27    H9      1.288902E-04   1.354587E-04   1.147867E-04
 28    H10    -7.684607E-06   7.751538E-05  -1.971835E-05
 29    C10    -5.673824E-05   2.082741E-05  -5.304689E-05
 30    H11    -5.201380E-05   9.993479E-06  -2.341748E-05
 31    H12     1.897933E-05   4.857679E-05   5.081694E-05
 32    H13     6.479873E-05  -8.475819E-05  -5.595551E-06
 33    H14    -1.880595E-05  -1.073763E-06  -6.258469E-05
 34    H15     5.874118E-04  -2.268905E-04  -1.203067E-04
 35    H16    -1.109102E-04   3.684404E-05   9.348339E-05
 36    H17    -7.911163E-05   3.786641E-04   2.379346E-04
-----------   -------------  -------------  -------------
   total       8.809291E-05   1.204375E-04  -4.889830E-04

 end of program der1b


 start of program geopt  11

 geometry optimization step 11
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:           2.6884E-05 *  (  5.0000E-05 )
 gradient maximum:        9.1225E-04 .  (  4.5000E-04 )
 gradient rms:            2.4166E-04 *  (  3.0000E-04 )
 step size:   0.01254  trust radius:   0.30000
 displacement maximum:    7.0448E-03 .  (  1.8000E-03 )
 displacement rms:        1.1353E-03 *  (  1.2000E-03 )
 predicted energy change:    -8.4547E-06    geom step:   1.2539E-
02    full step:   1.2539E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -4.8367E-05     y:    -5.2651E-04     z:    -2.6388E-04

 new geometry:
                              angstroms
 atom            x                y                z
 H1        1.0850921747     1.8755092669    -2.1965491526
```

```
 C1        1.4062084941      1.7561832750     -1.1757480190
 C2        2.2107414644      1.4390227011      1.4424643619
 C3        0.5908325386      1.0606464639     -0.2993300924
 C4        2.6202450422      2.2863714590     -0.7692810377
 C5        3.0155917584      2.1229057198      0.5450750098
 C6        0.9971866675      0.8997987549      1.0278528650
 C7       -0.7358799662      0.4816714766     -0.7412351434
 H3        3.2414331047      2.8186674605     -1.4669534120
 H4        3.9507487703      2.5319220510      0.8851919339
 H6        2.5318722206      1.3372322341      2.4607356785
 C16      -0.6487335495     -0.9400533005     -1.3004259650
 C8       -1.7348645937      0.5756493316      0.4281495668
 N2        0.1816163428      0.1781162701      1.9266990222
 C9       -1.1620060914     -0.0006065178      1.7099397489
 C11       0.7425796804     -0.3207253042      3.1737208278
 O1       -1.8662809930     -0.5501900183      2.5096769158
 C18      -0.6296527091     -3.5393536757     -2.3380197500
 C19      -1.6584645146     -1.3792395652     -2.1550052528
 C20       0.3736582472     -1.8237856179     -0.9816777131
 C21       0.3808893530     -3.1138997153     -1.4942937983
 C22      -1.6528728102     -2.6632812423     -2.6694371587
 H2       -2.4569640336     -0.7067872126     -2.4217729234
 H5        1.1753712384     -1.5107798074     -0.3386804980
 H7        1.1818385524     -3.7828989873     -1.2328996715
 H8       -2.4425309275     -2.9786884907     -3.3292818919
 H9       -0.6208387087     -4.5387043468     -2.7364236117
 H10      -1.1200077115      1.1079514568     -1.5409814595
 C10      -2.2056561335      2.0148901111      0.6922576077
 H11      -1.3767312470      2.6777121073      0.9166561551
 H12      -2.8966049060      2.0341262970      1.5273170640
 H13      -2.7182971815      2.4033646089     -0.1821731818
 H14      -2.6038873813     -0.0330943690      0.2154008615
 H15       1.7007590981     -0.7863838725      2.9806499142
 H16       0.0626423160     -1.0484296711      3.5816071177
 H17       0.8755339950      0.4765268612      3.8983337576

 nuclear repulsion energy.......  1415.606883182 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  11   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.349E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     88     88     89     87     83
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    182    183    195    181    183    192
171
  grid # 4      215    326    327    336    326    326    324
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     71     90     82     95     81
70
  grid # 2      118    118    112    100     90    104     90
79
  grid # 3      223    223    207    198    174    212    176
143
  grid # 4      224    223    207    342    312    390    293
273

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      261    184    183    182    184    185    215
211
  grid # 4      455    328    326    327    327    328    214
208

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     71     72     71
71
  grid # 2      118    118    118    106     79    109    111
110
  grid # 3      222    223    224    202    154    216    218
217
  grid # 4      223    224    224    199    290    216    220
219
```

```
  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2858
  grid # 2      110    110    108    111   3732
  grid # 3      214    213    212    217   7195
  grid # 4      207    211    209    218   9932

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                                 energy density   DIIS
       e  d  i  u  i                                 change change    error
       r  t  s  t  d     total energy

etot   1  N  N  1  U  -783.03321849990                       2.1E-05  1.2E-03
etot   2  Y  Y  4  M  -783.03329566222  7.7E-05  1.0E-05  4.6E-04
etot   3  Y  Y  4  M  -783.03330659391  1.1E-05  3.2E-06  1.2E-04
etot   4  Y  N  4  M  -783.03330700609  4.1E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.60688318196
   (E)  Total one-electron terms..... -3875.71614818851
   (I)  Total two-electron terms.....  1677.07595800046
   (L)  Electronic energy............. -2198.64019018805  (E+I)
   (N)  Total energy.................  -783.03330700609  (A+L)

 SCFE: SCF energy: HF    -783.03330700609 hartrees   iterations:
4


 HOMO energy:    -0.30332
 LUMO energy:     0.13259

  Orbital energies:
  -20.52366  -15.60107  -11.34422  -11.28712  -11.25586  -11.24895
  -11.24186  -11.24040  -11.24034  -11.23993  -11.23924  -11.23590
  -11.23099  -11.23078  -11.22961  -11.22897  -11.22746  -11.22669
  -11.22318   -1.39478   -1.26955   -1.16534   -1.14924   -1.10758
   -1.03271   -1.01977   -1.01809   -1.01131   -0.96088   -0.93324
   -0.85781   -0.84804   -0.83437   -0.82049   -0.79594   -0.74171
   -0.71074   -0.70030   -0.67043   -0.65046   -0.64815   -0.63596
   -0.63138   -0.61538   -0.61089   -0.60160   -0.59663   -0.58316
   -0.58076   -0.56482   -0.54945   -0.54503   -0.53545   -0.52345
   -0.52020   -0.50687   -0.49831   -0.49598   -0.48520   -0.46999
```

```
 -0.46481   -0.42095   -0.40859   -0.34195   -0.33186   -0.32295
 -0.30332    0.13259    0.13439    0.14410    0.14930    0.20785
  0.23183    0.23802    0.24543    0.25992    0.28875

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	1.509999E-05	-7.166566E-06	-7.375450E-06
2	C1	-1.403193E-04	-7.425558E-05	-1.456735E-06
3	C2	2.891177E-05	3.333228E-05	2.212443E-05
4	C3	5.810907E-05	6.259614E-05	-1.335858E-04
5	C4	-1.226377E-06	3.282838E-05	-9.614432E-05
6	C5	1.949114E-05	-1.214762E-05	1.645793E-04
7	C6	-1.303579E-05	-4.555087E-05	5.104680E-05
8	C7	-3.656073E-06	3.408986E-05	-9.098707E-05
9	H3	6.914848E-06	-2.595601E-06	1.331269E-06
10	H4	-2.452959E-05	6.190777E-06	1.587383E-05
11	H6	-1.101237E-05	9.965392E-06	2.318363E-05
12	C16	-1.159350E-04	-1.338367E-04	-1.735098E-04
13	C8	1.103544E-05	-5.062353E-05	2.676686E-05
14	N2	-1.495481E-04	1.293956E-04	-1.584863E-04
15	C9	1.120058E-05	1.006810E-04	-1.247190E-04
16	C11	-3.003755E-06	-2.935590E-05	-2.876516E-05
17	O1	-5.946309E-05	-6.440490E-05	5.928270E-05
18	C18	1.593486E-04	-1.018583E-04	1.158859E-04
19	C19	1.961710E-04	-5.289651E-05	9.435458E-05
20	C20	1.015188E-04	5.094383E-05	1.065040E-04
21	C21	-1.078614E-04	1.203866E-04	-9.521991E-05
22	C22	-2.206124E-04	1.774589E-04	-1.073953E-04
23	H2	-6.011433E-05	4.339600E-05	-4.340501E-05
24	H5	-1.329612E-04	-8.864390E-05	-2.088062E-04
25	H7	1.944857E-04	-1.209150E-04	1.712234E-05
26	H8	9.438265E-05	4.520749E-05	1.198306E-04
27	H9	5.751088E-05	2.061737E-05	3.817543E-05
28	H10	2.725181E-05	-9.019331E-06	-3.575937E-06
29	C10	6.106522E-05	4.533285E-05	-5.117092E-06
30	H11	-8.322761E-05	-6.001878E-05	-2.800072E-05
31	H12	-1.531791E-05	-2.247368E-06	-2.468381E-05

```
  32    H13     1.282610E-05  -6.343599E-06  -3.751185E-05
  33    H14     3.642051E-05   2.575478E-05  -2.038058E-05
  34    H15     1.302203E-04  -6.595604E-05   2.625067E-05
  35    H16    -1.722664E-05   1.717204E-05  -5.038503E-05
  36    H17     1.170832E-05   1.034583E-04   9.846561E-05
 -----------   -------------  -------------  -------------
    total       7.462175E-05   1.309715E-04  -4.587332E-04

  end of program der1b


  start of program geopt  12

  geometry optimization step 12
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -1.4274E-05 *  (  5.0000E-05 )
  gradient maximum:        3.4943E-04 *  (  4.5000E-04 )
  gradient rms:            9.7502E-05 *  (  3.0000E-04 )
  step size:   0.01215  trust radius:   0.30000
  displacement maximum:    6.4824E-03 .  (  1.8000E-03 )
  displacement rms:        1.1001E-03 *  (  1.2000E-03 )
  predicted energy change:    -2.9212E-06    geom step:   1.2151E-
02    full step:   1.2151E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.1589E-04     y:    -1.1907E-04     z:    -3.1836E-05

  new geometry:
                                angstroms
  atom            x                y                z
  H1        1.0874210424     1.8726767496    -2.1966991144
  C1        1.4076359920     1.7540999189    -1.1754995990
  C2        2.2103285271     1.4387751651     1.4439686467
  C3        0.5912764872     1.0599023605    -0.2990633807
  C4        2.6219041800     2.2838036755    -0.7684423765
  C5        3.0162712937     2.1212029846     0.5465915142
  C6        0.9967209296     0.8999135351     1.0286616086
  C7       -0.7354993908     0.4814207670    -0.7414582660
  H3        3.2440602389     2.8149272315    -1.4661033227
  H4        3.9515230447     2.5296883924     0.8870317539
  H6        2.5306265263     1.3376562691     2.4626884508
  C16      -0.6488642525    -0.9405067797    -1.3004612889
  C8       -1.7350603205     0.5762468038     0.4274478761
  N2        0.1802059148     0.1799571870     1.9277439932
```

```
  C9       -1.1631142305      0.0002261902      1.7096522898
  C11       0.7407712436     -0.3187777428      3.1754314820
  O1       -1.8674313305     -0.5502941385      2.5086197635
  C18      -0.6290397822     -3.5386971162     -2.3394572890
  C19      -1.6620976799     -1.3813001863     -2.1496964508
  C20       0.3776318664     -1.8218464172     -0.9875696398
  C21       0.3852029406     -3.1116046247     -1.5010657650
  C22      -1.6558386849     -2.6646009134     -2.6648769058
  H2       -2.4642945806     -0.7105462511     -2.4114926087
  H5        1.1817007206     -1.5076590403     -0.3486755518
  H7        1.1887025207     -3.7791158002     -1.2444160942
  H8       -2.4477505584     -2.9809918803     -3.3205967377
  H9       -0.6198143721     -4.5376904945     -2.7384639337
  H10      -1.1188644550      1.1076849813     -1.5415494224
  C10      -2.2053928127      2.0156943455      0.6909939541
  H11      -1.3765561397      2.6781177713      0.9160791304
  H12      -2.8970224903      2.0355085022      1.5254430647
  H13      -2.7168370781      2.4041393531     -0.1840580421
  H14      -2.6042485323     -0.0320723470      0.2144327156
  H15       1.7018027076     -0.7803438692      2.9851117766
  H16       0.0626661868     -1.0498218587      3.5797933091
  H17       0.8680497495      0.4778617252      3.9021196640

  nuclear repulsion energy.......  1415.566492597 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  12   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.352E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     88     88     89     87     84
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    182    183    194    181    183    192
171
```

```
  grid # 4      215    326    327    336    326    326    324
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     70     90     82     95     81
69
  grid # 2      118    118    112    100     90    105     90
80
  grid # 3      223    223    207    198    174    212    176
144
  grid # 4      224    223    207    342    312    390    293
272

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      261    184    183    182    184    185    214
211
  grid # 4      455    328    326    327    327    328    214
208

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     71     72     71
71
  grid # 2      118    118    118    106     79    109    111
110
  grid # 3      222    223    224    202    154    216    218
217
  grid # 4      223    224    224    199    290    216    220
219

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2857
  grid # 2      110    111    108    111   3735
  grid # 3      214    213    212    217   7194
  grid # 4      207    211    209    218   9931

  end of program grid


  start of program rwr
  end of program rwr
```

```
  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS     maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  1  U  -783.03322765343           1.8E-05  9.3E-04
etot  2  Y  Y  4  M  -783.03329023255  6.3E-05   8.9E-06  3.7E-04
etot  3  Y  Y  4  M  -783.03329907979  8.8E-06   2.7E-06  8.7E-05
etot  4  Y  N  4  M  -783.03329941947  3.4E-07   0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.56649259695
   (E)  Total one-electron terms..... -3875.64246018074
   (I)  Total two-electron terms.....  1677.04266816433
   (L)  Electronic energy............. -2198.59979201642  (E+I)
   (N)  Total energy.................  -783.03329941947  (A+L)

 SCFE: SCF energy: HF    -783.03329941947 hartrees   iterations:
4


 HOMO energy:    -0.30318
 LUMO energy:     0.13267

  Orbital energies:
  -20.52393  -15.60085  -11.34405  -11.28698  -11.25592  -11.24868
  -11.24161  -11.24025  -11.24006  -11.23997  -11.23917  -11.23593
  -11.23110  -11.23076  -11.22969  -11.22884  -11.22761  -11.22651
  -11.22312   -1.39481   -1.26939   -1.16523   -1.14917   -1.10751
   -1.03267   -1.01967   -1.01804   -1.01132   -0.96077   -0.93318
   -0.85777   -0.84802   -0.83428   -0.82041   -0.79593   -0.74163
   -0.71067   -0.70030   -0.67037   -0.65039   -0.64807   -0.63591
   -0.63127   -0.61536   -0.61085   -0.60151   -0.59660   -0.58321
   -0.58076   -0.56480   -0.54943   -0.54506   -0.53544   -0.52341
   -0.52012   -0.50680   -0.49830   -0.49591   -0.48524   -0.46984
   -0.46475   -0.42092   -0.40859   -0.34191   -0.33188   -0.32288
   -0.30318    0.13267    0.13438    0.14427    0.14926    0.20793
    0.23188    0.23799    0.24559    0.25997    0.28875

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr
```

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	9.550775E-06	1.862100E-06	1.298185E-05
2	C1	1.662934E-04	7.107516E-05	4.409654E-05
3	C2	-4.674395E-06	1.422456E-05	-3.297492E-05
4	C3	1.546377E-06	1.406442E-05	9.740599E-07
5	C4	-4.441744E-05	-5.447015E-05	9.556775E-05
6	C5	-4.772277E-05	2.057467E-05	-1.158832E-04
7	C6	4.498130E-05	8.357123E-05	4.897321E-05
8	C7	-1.433647E-05	3.448997E-05	5.589411E-05
9	H3	-1.201905E-05	1.738134E-06	1.251113E-05
10	H4	-5.282050E-05	1.168636E-05	-1.582899E-05
11	H6	-7.004268E-05	2.650758E-05	-9.432683E-05
12	C16	1.946571E-04	1.085630E-04	4.823569E-05
13	C8	-1.231475E-06	3.047010E-05	-1.146627E-05
14	N2	1.825481E-04	-6.266563E-05	-4.263682E-05
15	C9	1.316198E-04	-4.674712E-05	-7.785811E-05
16	C11	-3.344721E-05	1.338571E-04	-2.567368E-05
17	O1	-1.441563E-04	-5.546408E-05	1.069490E-04
18	C18	2.797816E-04	-9.327861E-06	1.327460E-04
19	C19	-9.724024E-05	2.700472E-04	1.468340E-05
20	C20	-1.903934E-04	-8.996130E-05	-6.072091E-05
21	C21	-3.568953E-04	1.065918E-04	-1.241310E-04
22	C22	-2.132966E-05	-1.139713E-04	-9.135987E-05
23	H2	2.599133E-04	-1.220062E-04	-2.101710E-05
24	H5	2.928700E-05	5.617728E-05	-3.449616E-06
25	H7	2.511586E-04	-1.538301E-04	9.375142E-05
26	H8	-1.690819E-04	-9.523210E-05	-1.515919E-04
27	H9	5.057564E-06	1.684253E-05	7.343854E-06
28	H10	8.823075E-06	1.402141E-05	-1.899764E-05
29	C10	3.579292E-05	1.881099E-06	-2.891656E-05
30	H11	1.550717E-05	-1.902495E-06	-2.175905E-05
31	H12	-3.390043E-05	-2.138714E-05	-4.421409E-05
32	H13	-3.275867E-05	2.412945E-05	-4.280185E-05
33	H14	2.475856E-05	-7.999042E-06	-7.114919E-06
34	H15	-1.620322E-04	5.566123E-05	-1.237246E-04
35	H16	-8.933291E-05	-9.802103E-05	8.553860E-05
36	H17	1.201349E-05	-9.911158E-06	-6.546425E-05
total		7.545714E-05	1.551397E-04	-4.616655E-04

end of program der1b

start of program geopt 13

```
  geometry optimization step 13
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:           7.5866E-06 *  (  5.0000E-05 )
  gradient maximum:        4.4609E-04 *  (  4.5000E-04 )
  gradient rms:            1.0872E-04 *  (  3.0000E-04 )
  step size:   0.00807  trust radius:   0.30000
  displacement maximum:    3.8703E-03 .  (  1.8000E-03 )
  displacement rms:        7.3097E-04 *  (  1.2000E-03 )
  predicted energy change:    -2.7443E-06    geom step:   8.0738E-
03    full step:   8.0738E-03
  molecular structure not yet converged...

  center of mass moved by:
     x:     7.9464E-05     y:     1.4919E-04     z:    -1.7791E-05

  new geometry:
                                angstroms
  atom            x                y                z
  H1         1.0873225631     1.8740356996    -2.1967669431
  C1         1.4075695345     1.7553611321    -1.1756107630
  C2         2.2101040554     1.4399897819     1.4437134769
  C3         0.5915520537     1.0604036397    -0.2994389538
  C4         2.6213261882     2.2858706647    -0.7683551621
  C5         3.0155548813     2.1234394678     0.5466161693
  C6         0.9970522390     0.9002002060     1.0281998385
  C7        -0.7351322176     0.4816902848    -0.7417311644
  H3         3.2431590682     2.8176725195    -1.4658220860
  H4         3.9503053051     2.5328687283     0.8872974977
  H6         2.5302626680     1.3389041983     2.4624047894
  C16       -0.6484959760    -0.9402089407    -1.3007668137
  C8        -1.7345167883     0.5757891140     0.4273753836
  N2         0.1811219234     0.1787728055     1.9267531824
  C9        -1.1623142954    -0.0004615067     1.7093620875
  C11        0.7420434031    -0.3206752566     3.1736974990
  O1        -1.8666783392    -0.5505674831     2.5086633502
  C18       -0.6305239831    -3.5395893382    -2.3376767482
  C19       -1.6602117605    -1.3801387888    -2.1523732841
  C20        0.3754361970    -1.8230566344    -0.9847378891
  C21        0.3823758086    -3.1132267411    -1.4972317720
  C22       -1.6556219849    -2.6643026021    -2.6662515461
  H2        -2.4597582434    -0.7081919123    -2.4171713098
  H5         1.1786085483    -1.5094515363    -0.3442970198
  H7         1.1852665442    -3.7814504098    -1.2384040781
  H8        -2.4471352063    -2.9803861643    -3.3234029244
  H9        -0.6220109882    -4.5389617150    -2.7358466293
```

```
  H10      -1.1187866345      1.1080633130     -1.5415617356
  C10      -2.2053318367      2.0149009697      0.6914469162
  H11      -1.3768830654      2.6771113800      0.9182989018
  H12      -2.8981092585      2.0336413654      1.5249667325
  H13      -2.7158621653      2.4042321355     -0.1838458554
  H14      -2.6034300371     -0.0328235863      0.2142993913
  H15       1.7014266015     -0.7846075109      2.9812736927
  H16       0.0627323523     -1.0499434529      3.5796876660
  H17       0.8728444505      0.4758884026      3.8997402002

  nuclear repulsion energy.......  1415.593187634 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  13   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.351E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     85     88     88     89     87     84
81
  grid # 2      116     95     95     98     97     97     95
90
  grid # 3      215    182    183    194    181    183    192
171
  grid # 4      215    326    327    336    326    326    324
315

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C11
  grid # 1       73     73     70     90     82     95     81
70
  grid # 2      118    118    112    100     90    105     90
80
  grid # 3      223    223    207    198    174    212    176
143
```

```
  grid # 4      224    223    207    342    312    390    293
272

  number of gridpoints:
     atom        O1    C18    C19    C20    C21    C22     H2
H5
  grid # 1      111     89     88     89     89     89     70
72
  grid # 2      122     97     96     96     97     97    113
112
  grid # 3      261    184    183    182    184    185    214
211
  grid # 4      455    328    326    327    327    328    214
208

  number of gridpoints:
     atom        H7     H8     H9    H10    C10    H11    H12
H13
  grid # 1       73     73     73     68     71     72     71
71
  grid # 2      118    118    118    106     79    109    111
110
  grid # 3      223    223    224    202    156    216    218
217
  grid # 4      223    224    224    199    290    216    220
219

  number of gridpoints:
     atom       H14    H15    H16    H17  total
  grid # 1       69     71     70     71   2858
  grid # 2      110    110    108    111   3734
  grid # 3      214    213    212    217   7196
  grid # 4      207    211    209    218   9931

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                                 energy density   DIIS
       e  d  i  u  i                                 change change    error
       r  t  s  t  d     total energy

etot   1  N  N  1  U  -783.03328122289                      1.2E-05  4.5E-04
etot   2  Y  Y  4  M  -783.03330080026  2.0E-05  5.1E-06  1.8E-04
etot   3  Y  Y  4  M  -783.03330222386  1.4E-06  1.6E-06  4.3E-05
etot   4  Y  N  4  M  -783.03330061721 -1.6E-06  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1415.59318763375
   (E)  Total one-electron terms..... -3875.69039243748
   (I)  Total two-electron terms.....  1677.06390418651
   (L)  Electronic energy..... -2198.62648825096  (E+I)
   (N)  Total energy.............  -783.03330061721  (A+L)

 SCFE: SCF energy: HF    -783.03330061721 hartrees   iterations:
4


 HOMO energy:    -0.30327
 LUMO energy:     0.13261

  Orbital energies:
 -20.52370  -15.60099  -11.34419  -11.28711  -11.25589  -11.24890
 -11.24185  -11.24036  -11.24019  -11.23995  -11.23925  -11.23590
 -11.23101  -11.23085  -11.22968  -11.22892  -11.22756  -11.22659
 -11.22315   -1.39477   -1.26952   -1.16531   -1.14921   -1.10757
  -1.03272   -1.01974   -1.01807   -1.01131   -0.96083   -0.93324
  -0.85781   -0.84806   -0.83433   -0.82045   -0.79596   -0.74170
  -0.71073   -0.70030   -0.67041   -0.65043   -0.64813   -0.63594
  -0.63132   -0.61538   -0.61086   -0.60158   -0.59662   -0.58319
  -0.58078   -0.56482   -0.54944   -0.54506   -0.53545   -0.52344
  -0.52016   -0.50686   -0.49829   -0.49598   -0.48520   -0.46995
  -0.46482   -0.42092   -0.40860   -0.34194   -0.33187   -0.32294
  -0.30327    0.13261    0.13437    0.14416    0.14926    0.20788
   0.23188    0.23803    0.24550    0.25995    0.28872

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1      1.657789E-05   2.544813E-06  -3.373277E-06
   2    C1     -5.172472E-06  -7.198763E-07   2.662704E-05
   3    C2     -2.609766E-05  -1.273136E-06  -1.548686E-05
   4    C3      5.593944E-05   3.750352E-05   1.920163E-05
```

5	C4	-2.477284E-05	-3.412211E-06	-1.076793E-05
6	C5	-6.307976E-06	8.702086E-07	7.345551E-06
7	C6	-1.374273E-06	1.055628E-05	-2.727527E-05
8	C7	1.015898E-05	-3.190100E-05	-1.022985E-05
9	H3	1.336100E-06	-1.441684E-06	6.076374E-07
10	H4	-1.290520E-05	7.027794E-06	3.121597E-06
11	H6	-2.254339E-05	1.122055E-05	-1.256761E-05
12	C16	-8.131633E-06	-4.342932E-06	-7.572126E-05
13	C8	1.817862E-05	-1.150560E-05	2.838909E-06
14	N2	-2.338560E-05	6.535674E-05	-7.314830E-05
15	C9	6.774645E-05	3.668454E-05	-1.093854E-04
16	C11	1.693877E-05	2.615144E-05	1.638908E-05
17	O1	-6.492795E-05	-5.926024E-05	4.135043E-05
18	C18	7.642989E-05	-1.422360E-06	8.289438E-05
19	C19	3.928692E-05	-8.296688E-05	1.736134E-05
20	C20	3.971244E-05	-3.795964E-05	2.286160E-05
21	C21	-2.588305E-05	-1.116993E-05	-9.306041E-05
22	C22	5.002591E-05	2.821340E-05	-4.644614E-05
23	H2	-7.356094E-05	6.991642E-05	-4.072812E-05
24	H5	3.312839E-06	-1.047249E-06	-5.457588E-05
25	H7	-4.291717E-05	1.650384E-05	-1.874377E-05
26	H8	9.272557E-05	3.095359E-05	6.278730E-05
27	H9	3.926596E-05	-7.364344E-06	1.004939E-05
28	H10	-4.037229E-06	3.030247E-06	-3.481205E-05
29	C10	-5.418467E-05	1.100297E-05	-4.638964E-05
30	H11	3.448245E-05	4.423627E-05	-2.277630E-05
31	H12	-1.976349E-05	8.491340E-06	-9.580463E-06
32	H13	-1.368800E-06	-7.604840E-06	-2.175043E-05
33	H14	-1.443588E-05	-1.042138E-05	-3.805171E-05
34	H15	-3.734217E-05	9.618748E-06	-1.005387E-05
35	H16	-1.264974E-05	-2.542782E-05	1.706236E-05
36	H17	-8.727188E-06	1.782744E-05	-5.884519E-06
total		7.162892E-05	1.384690E-04	-4.503108E-04

end of program der1b

start of program geopt 14

geometry optimization step 14
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format

energy change: -1.1977E-06 # (5.0000E-05)
gradient maximum: 1.5877E-04 * (4.5000E-04)
gradient rms: 3.9834E-05 # (3.0000E-04)

```
  step size:   0.00415  trust radius:   0.30000
  displacement maximum:    1.9381E-03 .  (  1.8000E-03 )
  displacement rms:        3.7594E-04 *  (  1.2000E-03 )
  predicted energy change:    -3.7460E-07    geom step:   4.1524E-
03    full step:   4.1524E-03

  ***********************************************************
  **           Geometry optimization complete              **
  ***********************************************************

  center of mass moved by:
     x:     0.0000E+00     y:     0.0000E+00     z:     0.0000E+00

  final geometry:
                                  angstroms
  atom            x                   y                   z
  H1         1.0873225631        1.8740356996       -2.1967669431
  C1         1.4075695345        1.7553611321       -1.1756107630
  C2         2.2101040554        1.4399897819        1.4437134769
  C3         0.5915520537        1.0604036397       -0.2994389538
  C4         2.6213261882        2.2858706647       -0.7683551621
  C5         3.0155548813        2.1234394678        0.5466161693
  C6         0.9970522390        0.9002002060        1.0281998385
  C7        -0.7351322176        0.4816902848       -0.7417311644
  H3         3.2431590682        2.8176725195       -1.4658220860
  H4         3.9503053051        2.5328687283        0.8872974977
  H6         2.5302626680        1.3389041983        2.4624047894
  C16       -0.6484959760       -0.9402089407       -1.3007668137
  C8        -1.7345167883        0.5757891140        0.4273753836
  N2         0.1811219234        0.1787728055        1.9267531824
  C9        -1.1623142954       -0.0004615067        1.7093620875
  C11        0.7420434031       -0.3206752566        3.1736974990
  O1        -1.8666783392       -0.5505674831        2.5086633502
  C18       -0.6305239831       -3.5395893382       -2.3376767482
  C19       -1.6602117605       -1.3801387888       -2.1523732841
  C20        0.3754361970       -1.8230566344       -0.9847378891
  C21        0.3823758086       -3.1132267411       -1.4972317720
  C22       -1.6556219849       -2.6643026021       -2.6662515461
  H2        -2.4597582434       -0.7081919123       -2.4171713098
  H5         1.1786085483       -1.5094515363       -0.3442970198
  H7         1.1852665442       -3.7814504098       -1.2384040781
  H8        -2.4471352063       -2.9803861643       -3.3234029244
  H9        -0.6220109882       -4.5389617150       -2.7358466293
  H10       -1.1187866345        1.1080633130       -1.5415617356
  C10       -2.2053318367        2.0149009697        0.6914469162
  H11       -1.3768830654        2.6771113800        0.9182989018
  H12       -2.8981092585        2.0336413654        1.5249667325
  H13       -2.7158621653        2.4042321355       -0.1838458554
  H14       -2.6034300371       -0.0328235863        0.2142993913
  H15        1.7014266015       -0.7846075109        2.9812736927
  H16        0.0627323523       -1.0499434529        3.5796876660
  H17        0.8728444505        0.4758884026        3.8997402002
```

```
 nuclear repulsion energy.......  1415.593187634 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  14   /
------------------------------------------------

 end of program geopt


 start of program post
 Writing a SPARTAN archive file
 end of program post

Total cpu seconds     user:    1010.859   user+sys:    1010.859
```

TRANS 2(EQ-EQ)

```
+-----------------------------------------------------------------
---+
  |  Jaguar version 3.5, release  42
|
  |
|
  |  Copyright 1991-1998 Schrodinger, Inc.
|
  |  All Rights Reserved.
|
  |
|
  |  Use of this program should be acknowledged in publications
as:    |
  |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.
|
  +-----------------------------------------------------------------
-----+

  start of program pre
  Job name: WF19262
  Executables used: D:\TITAN
  Temporary files : C:\Users\gfabr\AppData\Local\Temp\WF19262

  Input file comments:
    Molecule001
    This file created by Spartan

  basis set:              6-31G**
  net molecular charge:    0
  multiplicity:            1

  number of basis functions....          370

 Input geometry:
                                angstroms
  atom            x                  y                  z
  H1       -0.2632070000      1.4490920000     -1.9967150000
  C1       -0.1922820000      1.8630240000     -0.9827220000
  C2       -0.0220980000      2.9205440000      1.5809750000
  C3        0.1719080000      1.0263790000      0.0727920000
  C4       -0.4719140000      3.2060380000     -0.7672030000
  C5       -0.3957510000      3.7303800000      0.5177070000
  C6        0.2824390000      1.5682950000      1.3658120000
  C7        0.4868090000     -0.4220770000     -0.1784520000
  H3       -0.7560510000      3.8471180000     -1.6077730000
  H4       -0.6298660000      4.7854000000      0.6944020000
  H6        0.0270900000      3.3559530000      2.5867300000
  H7        1.5910980000     -0.4805290000     -0.3654610000
  C10      -0.2327600000     -0.9640970000     -1.3883640000
  C8        0.1607630000     -1.2828330000      1.0554990000
```

```
 C16       0.6386940000     -2.7123290000      0.8558630000
 H12      -0.9488380000     -1.2947100000      1.2079970000
 N2        0.6805350000      0.7433530000      2.4790550000
 C9        0.7675990000     -0.6722710000      2.3101260000
 C17       1.4070260000      1.4067250000      3.5864890000
 O1        1.2598680000     -1.3228910000      3.2197340000
 C11      -1.5277450000     -1.9970000000     -3.6375380000
 C12       0.5075810000     -1.4298780000     -2.4770510000
 C13      -1.6280170000     -1.0170630000     -1.4376170000
 C14      -2.2705290000     -1.5322850000     -2.5571970000
 C15      -0.1390100000     -1.9437780000     -3.5959010000
 H19       1.6031670000     -1.3936960000     -2.4510310000
 H20      -2.2181620000     -0.6441140000     -0.5919670000
 H21      -3.3643960000     -1.5710700000     -2.5874630000
 H22       0.4488190000     -2.3078780000     -4.4449180000
 H23      -2.0354520000     -2.4032150000     -4.5183150000
 H24       1.7287330000     -2.7639830000      0.7343660000
 H25       0.1839710000     -3.1519640000     -0.0420940000
 H11       0.3724790000     -3.3470310000      1.7108170000
 H2        2.0322840000      2.2323690000      3.2166710000
 H5        2.0608610000      0.7058760000      4.1249350000
 H8        0.6843540000      1.8141420000      4.3078120000

 Molecular weight:    251.13 amu

 Stoichiometry:        C17NH17O
 Molecular Point Group: C1
 Point Group used: C1
 nuclear repulsion energy.......  1389.422979657 hartrees

Non-default options chosen:
  Geometry will be optimized in redundant internal coordinates
  Initial Hessian: from previous calculation

 end of program pre


 start of program onee
 smallest eigenvalue of S:    3.501E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program hfig
 initial wavefunction generated automatically from atomic
wavefunctions

 Irreducible     Total no   No of occupied orbitals
 representation  orbitals   Shell_1  Shell_2    ...
 No Symm          368         67
 ------------------------
 Orbital occupation/shell    1.000
```

```
  end of program hfig


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       70     88     88     90     89     89     88
82
  grid # 2      112     96     96     98     97     97     99
90
  grid # 3      214    184    185    195    184    185    188
175
  grid # 4      221    328    329    343    328    328    330
309

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     69     92     82     74
68
  grid # 2      118    118    113    112    100     90     81
110
  grid # 3      224    223    209    210    191    175    150
213
  grid # 4      232    232    217    209    340    309    291
211

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       99     84     75    111     89     87     87
89
  grid # 2      107     94     80    123     97     95     95
95
  grid # 3      218    179    148    259    183    184    184
183
  grid # 4      396    299    279    454    326    328    328
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     70     73     73     73     71
71
```

```
  grid # 2       95    111    112    118    118    118    110
110
  grid # 3      183    214    213    224    224    224    218
214
  grid # 4      326    221    218    232    232    232    222
216

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       71     71     70     71   2882
  grid # 2      110    110    110    110   3745
  grid # 3      219    215    215    217   7223
  grid # 4      223    222    222    222  10081

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf
 number of electrons.........        134
 number of alpha electrons....         67
 number of beta electrons.....         67
 number of orbitals, total....        368
 number of core orbitals......         67
 number of open shell orbs....          0
 number of occupied orbitals..         67
 number of virtual orbitals...        301
 number of hamiltonians.......          1
 number of shells.............          1
 SCF type: HF

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                                 energy density   DIIS
       e  d  i  u  i                 total energy    change change    error

etot   1  N  N  5  M  -780.41224313436            4.8E-03  1.0E-01
etot   2  Y  Y  6  M  -782.69511415717  2.3E+00   1.9E-03  4.0E-02
etot   3  Y  Y  6  M  -782.94073970549  2.5E-01   8.7E-04  2.7E-02
etot   4  N  Y  2  U  -782.99814000209  5.7E-02   8.9E-04  1.3E-02
etot   5  Y  Y  6  M  -783.00909207368  1.1E-02   1.5E-03  8.3E-03
etot   6  N  Y  2  U  -783.01664101183  7.5E-03   1.6E-04  1.8E-03
etot   7  Y  Y  6  M  -783.01703738933  4.0E-04   5.9E-05  4.6E-04
etot   8  Y  Y  6  M  -783.01711453282  7.7E-05   1.2E-05  1.6E-04
etot   9  N  Y  2  U  -783.01696026698 -1.5E-04   5.3E-06  4.6E-05
etot  10  Y  Y  6  M  -783.01697008578  9.8E-06   3.6E-06  4.6E-05
etot  11  Y  N  6  M  -783.01697392616  3.8E-06   0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1389.42297965676
   (E)  Total one-electron terms..... -3823.49863253277
   (I)  Total two-electron terms.....  1651.05867894985
   (L)  Electronic energy............. -2172.43995358292  (E+I)
   (N)  Total energy.................  -783.01697392616  (A+L)

 SCFE: SCF energy: HF    -783.01697392616 hartrees   iterations:
11


 HOMO energy:    -0.29943
 LUMO energy:     0.12349

  Orbital energies:
 -20.53206  -15.59983  -11.35678  -11.28696  -11.26225  -11.25492
 -11.25425  -11.24685  -11.24272  -11.24254  -11.24180  -11.23975
 -11.23948  -11.23936  -11.23877  -11.23723  -11.23674  -11.23041
 -11.21648   -1.38068   -1.24500   -1.16986   -1.14163   -1.10881
  -1.03225   -1.01842   -1.01470   -1.00680   -0.94795   -0.92957
  -0.85828   -0.82994   -0.82652   -0.82570   -0.78631   -0.72997
  -0.71021   -0.69237   -0.67325   -0.65920   -0.63515   -0.63001
  -0.62525   -0.60999   -0.60710   -0.60168   -0.59516   -0.58712
  -0.56637   -0.55982   -0.54216   -0.53493   -0.52407   -0.52280
  -0.51209   -0.50181   -0.49625   -0.49569   -0.48431   -0.46978
  -0.46732   -0.42040   -0.40962   -0.34496   -0.33693   -0.32381
  -0.29943    0.12349    0.13307    0.13814    0.15110    0.18923
   0.23027    0.23577    0.24326    0.26113    0.26789

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x             y             z
 ----  -----   -------------  -------------  -------------
   1    H1      1.216512E-03   7.401360E-03   1.636917E-02
   2    C1     -9.484811E-04   1.628128E-03  -4.343009E-03
   3    C2      1.181325E-03   1.618374E-03   7.903980E-03
   4    C3     -3.711416E-03   1.669903E-02   3.097753E-03
   5    C4     -2.438866E-03   7.130554E-03  -7.777885E-03
   6    C5     -9.235378E-04   6.177562E-03  -1.025313E-03
```

7	C6	-2.933914E-03	-4.683387E-03	1.010828E-02
8	C7	1.580877E-02	-1.851436E-03	2.952512E-03
9	H3	3.410965E-03	-8.063187E-03	1.043779E-02
10	H4	2.988176E-03	-1.340038E-02	-1.623107E-03
11	H6	-7.528020E-04	-8.604488E-03	-1.520838E-02
12	H7	-1.951487E-02	-2.982938E-03	3.965787E-03
13	C10	4.092947E-03	-5.478590E-03	-1.212714E-02
14	C8	-9.341802E-03	2.741624E-03	3.404947E-03
15	C16	1.724932E-03	-2.041182E-02	3.267188E-03
16	H12	2.072100E-02	3.272786E-03	-1.121009E-03
17	N2	1.112626E-02	-1.661463E-02	-3.135123E-02
18	C9	1.704681E-02	1.994385E-02	5.960055E-02
19	C17	-1.454321E-03	-4.571388E-03	8.626210E-03
20	O1	-1.859035E-02	1.531711E-02	-4.140475E-02
21	C11	-2.260597E-03	-3.783296E-03	-8.452221E-03
22	C12	2.228845E-03	5.780684E-04	7.388006E-04
23	C13	-4.061735E-03	7.164229E-04	3.493603E-03
24	C14	-8.163763E-03	4.313684E-04	2.222082E-03
25	C15	2.861288E-03	-3.597021E-03	-8.324973E-03
26	H19	-1.463594E-02	-1.776008E-04	1.632400E-04
27	H20	7.530248E-03	-4.575028E-03	-1.245692E-02
28	H21	1.355474E-02	5.416067E-04	4.156136E-04
29	H22	-7.366234E-03	4.432473E-03	1.037037E-02
30	H23	6.318494E-03	5.082074E-03	1.090519E-02
31	H24	-8.493563E-03	2.254889E-03	1.816371E-03
32	H25	3.602734E-03	5.542729E-03	9.305871E-03
33	H11	3.330205E-03	7.343086E-03	-7.042697E-03
34	H2	-8.547816E-03	-9.569305E-03	-6.595902E-04
35	H5	-1.250518E-02	3.581786E-03	-1.156888E-02
36	H8	7.526786E-03	-3.130208E-03	-5.974848E-03
total		-3.741457E-04	9.401775E-04	-1.296659E-03

```
 end of program der1b


 start of program geopt   1

 geometry optimization step  1
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3004235
  Cos(theta):   0.8097400

  Final level shift:  -7.1129141E-02

 gradient maximum:        4.6421E-02 .  (  4.5000E-04 )
 gradient rms:            1.0915E-02 .  (  3.0000E-04 )
 step size:   0.30042  trust radius:   0.30000
```

```
  displacement maximum:    1.0149E-01 .  (  1.8000E-03 )
  displacement rms:        2.7199E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.7874E-02    geom step:   3.0042E-
01    full step:   3.0042E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     2.3991E-02     y:     8.7476E-03     z:    -2.7017E-02

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -0.3233054359      1.5524589487     -1.9475020147
  C1       -0.2239662350      1.9217702639     -0.9451958548
  C2        0.0074050266      2.9097785253      1.5879783273
  C3        0.1623146593      1.0577122290      0.0682075255
  C4       -0.4960147779      3.2580678993     -0.7111671030
  C5       -0.3895940860      3.7447732384      0.5654029444
  C6        0.3103170107      1.5730729949      1.3468583504
  C7        0.4689769921     -0.4102457139     -0.1923143171
  H3       -0.7945944805      3.9009270237     -1.5195083551
  H4       -0.6172974209      4.7742179789      0.7762559786
  H6        0.0823911603      3.3099165095      2.5787107779
  H7        1.5428708771     -0.4874998146     -0.3782428806
  C10      -0.2397527156     -0.9757213662     -1.4123366481
  C8        0.1757762685     -1.2472295649      1.0693336547
  C16       0.5950591169     -2.7041935058      0.9470091322
  H12      -0.8912175798     -1.2129158036      1.2634904340
  N2        0.7333627481      0.7492084767      2.4193894183
  C9        0.8172149517     -0.6323258527      2.3048138033
  C17       1.3632818307      1.3587829239      3.5846685076
  O1        1.3098242984     -1.3190152768      3.1517759515
  C11      -1.5329017608     -2.0495830653     -3.6436011536
  C12       0.4866093356     -1.4335773591     -2.4974137514
  C13      -1.6296037965     -1.0600231967     -1.4613723850
  C14      -2.2704711789     -1.5933371198     -2.5635188934
  C15      -0.1506004056     -1.9668753319     -3.6081287347
  H19       1.5600066926     -1.3802941893     -2.4848359129
  H20      -2.2173860238     -0.7021409676     -0.6342774474
  H21      -3.3432905328     -1.6553136130     -2.5813994550
  H22       0.4300347654     -2.3181277140     -4.4439246156
  H23      -2.0283452018     -2.4653000982     -4.5039411372
  H24       1.6691163104     -2.7809876315      0.7939142418
  H25       0.0914571248     -3.1650405823      0.1057695913
  H11       0.3534798976     -3.2570268342      1.8479164175
  H2        2.0068930016      2.1706348652      3.2681350390
  H5        1.9232845083      0.6031705140      4.1186331865
  H8        0.6016287406      1.7656350632      4.2451007145

  nuclear repulsion energy.......  1394.427370292 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   1   /
```

```
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.205E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     86     86     92     89     88     84
82
  grid # 2      113     96     96    100     97     97     94
90
  grid # 3      213    182    183    193    182    183    186
175
  grid # 4      212    327    327    342    326    328    326
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     67     90     81     73
69
  grid # 2      118    118    113    106    100     90     80
108
  grid # 3      223    223    208    208    193    172    151
212
  grid # 4      223    223    207    207    339    314    288
206

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       98     82     72    111     89     86     87
89
  grid # 2      107     92     79    123     97     95     95
95
  grid # 3      216    175    144    255    182    182    183
183
  grid # 4      393    295    274    449    326    326    327
326
```

```
  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     71     73     73     73     71
71
  grid # 2       96    111    113    118    118    118    108
110
  grid # 3      183    213    212    222    222    223    217
215
  grid # 4      326    212    209    223    224    224    220
211

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       70     72     71     71   2866
  grid # 2      108    109    106    111   3725
  grid # 3      217    216    214    217   7178
  grid # 4      218    212    212    217   9931

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                                 energy density   DIIS
       e  d  i  u  i                 total energy    change change    error

etot   1  N  N  2  U  -783.01661463221                      3.4E-04  6.1E-03
etot   2  Y  Y  6  M  -783.03038147071  1.4E-02  1.2E-04  1.8E-03
etot   3  N  Y  2  U  -783.03172559975  1.3E-03  4.2E-05  7.6E-04
etot   4  Y  Y  6  M  -783.03188003352  1.5E-04  1.8E-05  3.0E-04
etot   5  Y  Y  6  M  -783.03190512950  2.5E-05  6.4E-06  1.0E-04
etot   6  Y  Y  6  M  -783.03191178670  6.7E-06  2.6E-06  3.8E-05
etot   7  Y  N  6  M  -783.03191372217  1.9E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1394.42737029176
   (E)  Total one-electron terms..... -3833.33263364082
   (I)  Total two-electron terms.....  1655.87334962689
   (L)  Electronic energy............. -2177.45928401393  (E+I)
   (N)  Total energy.................  -783.03191372217  (A+L)

 SCFE: SCF energy: HF    -783.03191372217 hartrees   iterations:
7
```

```
HOMO energy:    -0.30202
LUMO energy:     0.12785

 Orbital energies:
 -20.53029  -15.59887  -11.34783  -11.28415  -11.25476  -11.25190
 -11.24308  -11.24165  -11.24087  -11.23591  -11.23560  -11.23408
 -11.23331  -11.23300  -11.23287  -11.23277  -11.23070  -11.22491
 -11.20745   -1.39943   -1.26530   -1.17017   -1.15031   -1.10778
  -1.03237   -1.02208   -1.01867   -1.01438   -0.95675   -0.93293
  -0.85881   -0.83612   -0.83171   -0.83102   -0.79162   -0.74064
  -0.71305   -0.69668   -0.68069   -0.66472   -0.63912   -0.63699
  -0.63065   -0.61617   -0.61323   -0.60515   -0.59911   -0.58875
  -0.57055   -0.56188   -0.55102   -0.53839   -0.52863   -0.52056
  -0.51449   -0.50517   -0.50002   -0.49717   -0.48540   -0.47072
  -0.46865   -0.42214   -0.41186   -0.34350   -0.33711   -0.32530
  -0.30202    0.12785    0.13651    0.14169    0.15262    0.20401
   0.23660    0.24061    0.25330    0.26312    0.27316

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1      2.946812E-04  -2.480286E-03  -3.119281E-04
  2    C1     -1.414020E-03   1.221586E-03  -4.758878E-03
  3    C2      2.860683E-03   3.244940E-04   5.780297E-03
  4    C3     -1.381596E-03  -2.778642E-03  -8.769305E-03
  5    C4     -8.018140E-04  -2.704573E-03  -9.180670E-03
  6    C5      3.178814E-05   5.398674E-03   5.978645E-03
  7    C6     -4.975090E-03  -8.522176E-04   1.362908E-02
  8    C7      4.597344E-03  -1.047195E-03   1.154727E-03
  9    H3     -5.355948E-05  -6.721349E-04  -7.360825E-04
 10    H4      2.676963E-04   4.328616E-04   9.426712E-04
 11    H6     -8.083509E-05  -5.141850E-04   1.614840E-03
 12    H7     -1.493302E-03  -9.494878E-05   7.622630E-05
 13    C10    -1.719876E-03   1.366604E-03   2.081013E-03
 14    C8      7.139626E-04   3.063500E-03   3.111099E-03
 15    C16     2.113760E-03  -4.534018E-03  -1.947305E-03
```

```
 16    H12    -3.434140E-03   1.541293E-03  -2.685647E-04
 17    N2      1.223482E-02  -1.498630E-02  -4.726356E-03
 18    C9     -6.460669E-03   1.214446E-02  -4.601785E-03
 19    C17    -6.827225E-03   2.188684E-03   2.354379E-03
 20    O1      1.878983E-03   3.567462E-03   3.944199E-03
 21    C11     3.522130E-03  -1.119456E-03  -2.784678E-03
 22    C12     1.378590E-03  -1.090514E-03  -3.039976E-03
 23    C13    -9.024747E-04   2.247939E-04   1.193181E-03
 24    C14    -5.194442E-04   7.994157E-05   9.485047E-04
 25    C15    -3.144207E-03  -9.882206E-04  -2.116226E-03
 26    H19     1.384487E-03   4.178748E-04   6.565263E-04
 27    H20     1.319449E-04   4.942550E-04  -3.116216E-05
 28    H21    -1.004921E-03   3.351855E-04   2.751131E-04
 29    H22     1.892500E-04   2.242599E-04   6.256668E-04
 30    H23     5.597755E-05   1.781865E-04   3.582990E-04
 31    H24    -1.553314E-03  -6.139467E-04  -2.084405E-04
 32    H25     6.294887E-04  -8.646965E-04   4.857943E-04
 33    H11     1.899193E-04   2.082679E-03  -1.785110E-03
 34    H2      2.323944E-03  -1.732962E-03   9.728723E-04
 35    H5     -1.396116E-03   3.130499E-03  -3.132728E-03
 36    H8      2.278221E-03  -4.086534E-04   1.417418E-03
-----------   -------------  -------------  -------------
   total      -8.493522E-05   9.343482E-04  -7.986462E-04

 end of program der1b


 start of program geopt   2

 geometry optimization step  2
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3000065
  Cos(theta):   0.4060511

  Final level shift:  -1.5786604E-02

 energy change:          -1.4940E-02 .  (  5.0000E-05 )
 gradient maximum:        1.5589E-02 .  (  4.5000E-04 )
 gradient rms:            3.1363E-03 .  (  3.0000E-04 )
 step size:   0.29998  trust radius:   0.30000
 displacement maximum:    1.7545E-01 .  (  1.8000E-03 )
 displacement rms:        2.7159E-02 .  (  1.2000E-03 )
 predicted energy change:    -2.8203E-03    geom step:   2.9998E-
01    full step:   2.9998E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:     1.7179E-02     y:     3.6276E-03     z:    -1.0908E-02
```

```
 new geometry:
                                angstroms
 atom            x                  y                  z
 H1       -0.3996483143      1.5369179461     -1.9363770706
 C1       -0.2730432873      1.9217832495     -0.9446919708
 C2        0.0360693755      2.9144428262      1.6102354164
 C3        0.1495351132      1.0633782155      0.0604088388
 C4       -0.5399974571      3.2591863390     -0.6948484360
 C5       -0.3929202203      3.7473670502      0.5928367385
 C6        0.3347320222      1.5783706301      1.3511142379
 C7        0.4651728514     -0.4083799650     -0.1984790275
 H3       -0.8666947368      3.8999357505     -1.4916504543
 H4       -0.6134795246      4.7752942710      0.8141777273
 H6        0.1351042536      3.3089667482      2.6003830771
 H7        1.5331740386     -0.4879411432     -0.3854093240
 C10      -0.2435106964     -0.9805386954     -1.4188333608
 C8        0.1657996569     -1.2267682839      1.0760094583
 C16       0.5491856917     -2.6989038081      0.9561364962
 H12      -0.9015233051     -1.1551804396      1.2764599388
 N2        0.8228637823      0.7514992683      2.3803398805
 C9        0.8383065184     -0.6098634052      2.2930333040
 C17       1.3541778128      1.3533257907      3.6070993777
 O1        1.3243280291     -1.2920135116      3.1533606174
 C11      -1.5253313347     -2.0783442760     -3.6554667787
 C12       0.4845809708     -1.4379766487     -2.5084357534
 C13      -1.6302601779     -1.0758006953     -1.4685555075
 C14      -2.2649308215     -1.6210670026     -2.5721700794
 C15      -0.1490955569     -1.9825524836     -3.6212175039
 H19       1.5580285539     -1.3722426757     -2.4914288360
 H20      -2.2210236799     -0.7150790993     -0.6475211221
 H21      -3.3378524882     -1.6875776664     -2.5875264862
 H22       0.4388408846     -2.3292597046     -4.4507514522
 H23      -2.0207302030     -2.5007353703     -4.5092025274
 H24       1.6126357849     -2.8025872921      0.7596910395
 H25      -0.0003772391     -3.1666863820      0.1462627778
 H11       0.3325329569     -3.2200891237      1.8786962291
 H2        2.0504101170      2.1442691948      3.3484708458
 H5        1.8558065962      0.5861685851      4.1785594754
 H8        0.5548312631      1.7729272301      4.2217791524

 nuclear repulsion energy.......  1393.103272287 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   2   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.360E-04
 number of canonical orbitals.....          368
```

```
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     87     89     88     89     89     86
82
  grid # 2      113     96     96     98     97     97     93
91
  grid # 3      213    184    184    192    183    184    191
171
  grid # 4      212    327    329    340    328    328    326
315

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     67     92     82     73
68
  grid # 2      118    118    111    106    100     90     80
111
  grid # 3      223    223    207    211    192    175    150
213
  grid # 4      224    223    206    208    339    310    288
209

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       96     82     72    111     89     87     87
89
  grid # 2      104     92     78    123     97     95     95
95
  grid # 3      214    176    146    256    181    182    182
183
  grid # 4      393    295    276    448    326    326    327
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     71     73     73     73     71
71
  grid # 2       96    111    113    118    118    118    108
110
```

```
  grid # 3      181    213    212    223    223    224    218
215
  grid # 4      326    213    209    223    224    224    219
214

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       70     71     70     71   2868
  grid # 2      108    111    105    111   3721
  grid # 3      218    217    214    215   7189
  grid # 4      215    215    208    221   9940

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
       r  t  s  t  d     total energy   change  change    error

etot   1  N  N  2  U  -783.02396153890           2.5E-04  8.1E-03
etot   2  Y  Y  6  M  -783.03253844321  8.6E-03  9.8E-05  2.0E-03
etot   3  N  Y  2  U  -783.03347133509  9.3E-04  2.7E-05  4.6E-04
etot   4  Y  Y  6  M  -783.03354015458  6.9E-05  1.4E-05  2.8E-04
etot   5  Y  Y  6  M  -783.03356027524  2.0E-05  4.8E-06  1.3E-04
etot   6  Y  N  6  M  -783.03356181976  1.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1393.10327228684
   (E)  Total one-electron terms..... -3830.69474562281
   (I)  Total two-electron terms.....  1654.55791151620
   (L)  Electronic energy............. -2176.13683410660  (E+I)
   (N)  Total energy.................  -783.03356181976  (A+L)

 SCFE: SCF energy: HF    -783.03356181976 hartrees   iterations:
6


 HOMO energy:    -0.29940
 LUMO energy:     0.12704

  Orbital energies:
  -20.52541  -15.60144  -11.34539  -11.28611  -11.25740  -11.25167
  -11.24347  -11.24239  -11.24230  -11.23672  -11.23623  -11.23579
  -11.23393  -11.23383  -11.23319  -11.23280  -11.23220  -11.22706
```

```
-11.20725   -1.39706   -1.26918   -1.16880   -1.14742   -1.10650
 -1.03080   -1.01943   -1.01784   -1.01531   -0.95999   -0.93253
 -0.85923   -0.83920   -0.83194   -0.82944   -0.79054   -0.74325
 -0.71226   -0.69652   -0.68087   -0.66436   -0.64103   -0.63702
 -0.62861   -0.61710   -0.61129   -0.60385   -0.59901   -0.58754
 -0.57038   -0.56148   -0.54947   -0.54029   -0.52930   -0.51969
 -0.51383   -0.50497   -0.50000   -0.49697   -0.48412   -0.46944
 -0.46811   -0.42155   -0.41221   -0.34350   -0.33551   -0.32674
 -0.29940    0.12704    0.13573    0.14142    0.15107    0.20583
  0.23649    0.24157    0.25374    0.26146    0.27434

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.135083E-04	-6.286168E-04	-1.873390E-03
2	C1	-6.687103E-05	1.272085E-03	3.376783E-03
3	C2	1.499807E-03	-2.401160E-03	-1.430940E-03
4	C3	1.182469E-03	-1.603749E-05	2.695036E-04
5	C4	7.283216E-04	-6.322224E-04	3.674155E-03
6	C5	-6.550520E-04	-1.490156E-03	-4.181160E-03
7	C6	-5.047128E-03	2.828756E-04	-2.625254E-03
8	C7	-1.344135E-03	2.038558E-03	1.464306E-03
9	H3	-3.101026E-04	1.009778E-03	-8.461383E-04
10	H4	-2.484883E-04	1.108742E-03	6.235260E-06
11	H6	4.510337E-04	5.211168E-04	1.026954E-03
12	H7	2.020119E-03	1.971991E-04	2.543763E-04
13	C10	2.189480E-03	-2.636749E-04	-4.225802E-04
14	C8	7.482780E-04	4.611776E-04	-1.449033E-03
15	C16	-3.769310E-04	-1.057411E-03	-9.703906E-04
16	H12	-1.103899E-03	2.426389E-04	1.347781E-04
17	N2	4.829313E-03	4.616149E-03	8.912314E-03
18	C9	3.445797E-04	-5.608668E-03	-7.134717E-04
19	C17	-2.991962E-03	1.110806E-03	-5.145103E-04
20	O1	-1.413909E-03	-1.207804E-04	-1.398680E-04
21	C11	-1.568916E-03	9.463753E-04	2.340554E-03
22	C12	-4.802509E-04	-3.477659E-04	-9.896520E-04
23	C13	-2.955854E-03	-1.538581E-03	-3.242750E-03
24	C14	5.462180E-04	6.582222E-04	1.378059E-03

```
  25    C15     2.832434E-03   1.522608E-03   3.031645E-03
  26    H19     8.693128E-04  -8.789744E-05  -2.374359E-04
  27    H20    -1.030753E-03   5.361218E-04   1.077201E-03
  28    H21    -7.931738E-04   5.687433E-06  -7.818673E-05
  29    H22     8.058104E-04  -4.179961E-04  -9.483579E-04
  30    H23    -7.510830E-04  -5.576272E-04  -1.255846E-03
  31    H24    -7.739141E-04  -3.586916E-04  -9.097780E-05
  32    H25     1.010692E-03   2.653832E-04   1.233505E-03
  33    H11     2.077589E-04  -2.002025E-06  -6.036245E-04
  34    H2     -3.738108E-04  -1.168466E-03   1.214606E-03
  35    H5     -9.437069E-04   2.451644E-03  -3.559883E-03
  36    H8      2.838689E-03  -1.928587E-03  -3.607719E-03
 -----------   -------------  -------------  -------------
    total      -3.391319E-04   6.208253E-04  -3.861949E-04

  end of program der1b


  start of program geopt   3

  geometry optimization step  3
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -1.6481E-03 .  (  5.0000E-05 )
  gradient maximum:        6.4471E-03 .  (  4.5000E-04 )
  gradient rms:            1.6599E-03 .  (  3.0000E-04 )
  step size:   0.19130  trust radius:   0.30000
  displacement maximum:    9.0660E-02 .  (  1.8000E-03 )
  displacement rms:        1.7320E-02 .  (  1.2000E-03 )
  predicted energy change:    -7.7858E-04    geom step:   1.9130E-
01    full step:   1.9130E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.8114E-02     y:    -8.1882E-04     z:     1.1302E-02

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -0.4810339862     1.5257582202    -1.9167092479
  C1       -0.3339796612     1.9181339032    -0.9275601628
  C2        0.0423770935     2.9175841717     1.6233004643
  C3        0.1189373497     1.0655750957     0.0689496770
  C4       -0.5984003844     3.2543896566    -0.6719346318
  C5       -0.4156742103     3.7473700122     0.6122914681
  C6        0.3250922697     1.5800317689     1.3603772029
  C7        0.4527981714    -0.4006110329    -0.1860537094
  H3       -0.9449965946     3.8951269503    -1.4628265883
```

```
 H4       -0.6305146138      4.7772795814      0.8361541113
 H6        0.1722817442      3.3105569415      2.6116210618
 H7        1.5262446133     -0.4724952140     -0.3510294500
 C10      -0.2284305219     -0.9781573592     -1.4204445662
 C8        0.1276214510     -2.1668574902      1.0828646874
 C16       0.4921751453     -2.6969247138      0.9600671814
 H12      -0.9430416440     -1.1247018016      1.2692857665
 N2        0.8437067692      0.7545844969      2.3799616384
 C9        0.8036421222     -0.6119377014      2.3011783548
 C17       1.4726859672      1.3538279381      3.5369585070
 O1        1.2390859482     -1.2996421355      3.1843107993
 C11      -1.4532785525     -2.0845951657     -3.6776755845
 C12       0.5307447023     -1.4479703913     -2.4850535303
 C13      -1.6177973586     -1.0650498493     -1.5067746423
 C14      -2.2241218692     -1.6138374925     -2.6209750778
 C15      -0.0759791970     -1.9979890625     -3.6073514470
 H19       1.6052069831     -1.3858525141     -2.4350342566
 H20      -2.2281959107     -0.6877537230     -0.7050068944
 H21      -3.2976678299     -1.6713595500     -2.6685688827
 H22       0.5328768331     -2.3578550922     -4.4178188995
 H23      -1.9272904951     -2.5111691737     -4.5436378292
 H24       1.5516876072     -2.8163314176      0.7710831785
 H25      -0.0548617301     -3.1543687675      0.1488952484
 H11       0.2639130229     -3.2170830264      1.8769975447
 H2        2.1177939383      2.1663984479      3.2394997253
 H5        2.0589537749      0.5959601453      4.0127485234
 H8        0.7382133693      1.7298099622      4.2350977493

 nuclear repulsion energy.......  1393.760434242 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   3   /
 ------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.378E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H1     C1     C2     C3     C4     C5     C6
C7
```

grid # 1	71	86	89	88	89	89	87
82							
grid # 2	113	96	96	98	97	97	94
91							
grid # 3	213	184	184	192	183	184	190
175							
grid # 4	213	327	328	341	328	328	327
313							

number of gridpoints:

atom	H3	H4	H6	H7	C10	C8	C16
H12							
grid # 1	73	73	70	67	92	81	71
68							
grid # 2	118	118	112	106	100	91	79
110							
grid # 3	223	223	208	211	192	173	153
213							
grid # 4	224	223	208	208	337	313	288
208							

number of gridpoints:

atom	N2	C9	C17	O1	C11	C12	C13
C14							
grid # 1	97	81	69	111	89	87	87
89							
grid # 2	106	91	79	122	97	95	95
95							
grid # 3	209	176	142	256	181	183	183
183							
grid # 4	391	292	270	449	326	326	326
326							

number of gridpoints:

atom	C15	H19	H20	H21	H22	H23	H24
H25							
grid # 1	89	73	71	73	73	73	71
71							
grid # 2	96	111	113	118	118	118	108
110							
grid # 3	181	213	212	223	223	224	218
215							
grid # 4	326	213	211	223	224	224	217
212							

number of gridpoints:

atom	H11	H2	H5	H8	total
grid # 1	70	71	70	71	2862
grid # 2	108	111	107	111	3725
grid # 3	218	215	212	217	7185
grid # 4	214	213	209	215	9921

```
  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  2  U  -783.02286010499           2.3E-04  7.8E-03
etot  2  Y  Y  6  M  -783.03264117030  9.8E-03  1.1E-04  2.2E-03
etot  3  N  Y  2  U  -783.03377403359  1.1E-03  2.5E-05  4.9E-04
etot  4  Y  Y  6  M  -783.03381452766  4.0E-05  1.1E-05  2.4E-04
etot  5  Y  Y  6  M  -783.03382670949  1.2E-05  3.4E-06  9.0E-05
etot  6  Y  N  6  M  -783.03382610167 -6.1E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1393.76043424191
   (E)  Total one-electron terms..... -3831.98161857135
   (I)  Total two-electron terms.....  1655.18735822777
   (L)  Electronic energy............. -2176.79426034358  (E+I)
   (N)  Total energy.................  -783.03382610167  (A+L)

 SCFE: SCF energy: HF    -783.03382610167 hartrees   iterations:
6


 HOMO energy:    -0.29979
 LUMO energy:     0.12673

  Orbital energies:
  -20.52581  -15.60027  -11.34577  -11.28550  -11.25255  -11.25155
  -11.24410  -11.24330  -11.24259  -11.23777  -11.23670  -11.23623
  -11.23441  -11.23430  -11.23381  -11.23348  -11.23288  -11.22814
  -11.20684   -1.39706   -1.27012   -1.16894   -1.14730   -1.10682
   -1.03052   -1.01961   -1.01827   -1.01547   -0.96174   -0.93277
   -0.85958   -0.83870   -0.83166   -0.82951   -0.79016   -0.74337
   -0.71244   -0.69682   -0.68132   -0.66484   -0.64236   -0.63731
   -0.62812   -0.61778   -0.61201   -0.60438   -0.60105   -0.58872
   -0.56985   -0.56144   -0.54940   -0.54017   -0.52908   -0.52156
   -0.51436   -0.50511   -0.49970   -0.49682   -0.48415   -0.46952
   -0.46852   -0.42042   -0.41259   -0.34362   -0.33586   -0.32674
   -0.29979    0.12673    0.13548    0.14114    0.15127    0.20370
    0.23597    0.24182    0.25305    0.26258    0.27471

  end of program scf
```

start of program der1a
end of program der1a

start of program rwr
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	1.314618E-04	9.671254E-04	1.357224E-04
2	C1	6.049239E-04	-7.423106E-04	2.267646E-03
3	C2	-5.586920E-04	-2.195561E-03	-2.866624E-03
4	C3	1.724278E-03	9.133594E-04	3.740969E-03
5	C4	6.232382E-04	1.998658E-03	5.298173E-03
6	C5	-5.388110E-04	-2.128700E-03	-4.468745E-03
7	C6	-1.933875E-03	2.555391E-04	-5.389692E-03
8	C7	-3.113262E-03	1.337530E-03	-1.467681E-04
9	H3	-1.260533E-04	2.541355E-04	3.724507E-04
10	H4	3.644154E-05	2.435567E-04	-3.499960E-04
11	H6	-8.917927E-05	9.206511E-04	4.131060E-04
12	H7	1.059598E-03	2.667708E-04	5.567965E-04
13	C10	1.542757E-03	-2.641351E-04	-6.815840E-04
14	C8	2.542714E-04	-5.219931E-04	-3.295019E-03
15	C16	-1.259003E-03	2.188755E-03	1.362962E-03
16	H12	6.800257E-04	-5.669417E-04	4.131426E-04
17	N2	2.132449E-05	-5.914599E-04	-1.062572E-02
18	C9	-1.768636E-03	-1.696436E-03	6.599596E-03
19	C17	9.235317E-04	7.418552E-04	2.358667E-03
20	O1	7.285951E-04	2.708922E-04	-1.981693E-03
21	C11	-1.411606E-03	2.066161E-04	6.762982E-04
22	C12	-8.796131E-04	9.770619E-04	2.148481E-03
23	C13	7.816499E-04	2.121748E-04	-1.527311E-04
24	C14	3.805430E-04	-3.103672E-04	-9.273715E-04
25	C15	9.994358E-04	2.473726E-04	7.605118E-04
26	H19	-6.063186E-04	-3.012661E-04	-5.747651E-04
27	H20	-5.654176E-05	-2.808744E-04	7.073214E-05
28	H21	8.476526E-05	-1.532948E-04	-1.852192E-04
29	H22	-1.040160E-04	-4.863888E-05	-3.798131E-04
30	H23	-7.441393E-05	-1.152353E-04	-2.505133E-04
31	H24	1.825881E-03	-5.690465E-05	-6.010807E-04
32	H25	-8.969310E-04	-7.389695E-04	-1.181854E-03
33	H11	-4.141372E-04	-7.905244E-04	1.401117E-03
34	H2	8.667737E-04	1.994440E-03	-2.484903E-03
35	H5	2.107900E-03	-2.477809E-03	4.488441E-03
36	H8	-1.739512E-03	5.914137E-04	3.020846E-03

```
 -----------   -------------  -------------  -------------
    total      -1.932030E-04   6.064846E-04  -4.584316E-04

  end of program der1b


  start of program geopt   4

  geometry optimization step  4
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3003236
   Cos(theta):   0.2649517

   Final level shift:  -1.4878527E-03

  energy change:          -2.6428E-04 .  (  5.0000E-05 )
  gradient maximum:        7.2633E-03 .  (  4.5000E-04 )
  gradient rms:            1.6929E-03 .  (  3.0000E-04 )
  step size:   0.30029  trust radius:   0.30000
  displacement maximum:    1.6195E-01 .  (  1.8000E-03 )
  displacement rms:        2.7187E-02 .  (  1.2000E-03 )
  predicted energy change:    -8.1092E-04    geom step:   3.0029E-
01    full step:   3.0029E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.4205E-02     y:    -2.6951E-04     z:    -8.0476E-03

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -0.5741894742      1.5311294878     -1.8959211973
  C1       -0.3872706475      1.9180168576     -0.9092972026
  C2        0.0928444108      2.9243636689      1.6023522802
  C3        0.1069356853      1.0682445418      0.0698798477
  C4       -0.6438703943      3.2545368402     -0.6549007642
  C5       -0.4073826722      3.7516896589      0.6081636780
  C6        0.3593469855      1.5870256104      1.3420964774
  C7        0.4351587469     -0.3968759049     -0.1810498442
  H3       -1.0244407892      3.8903505694     -1.4368993563
  H4       -0.6086934411      4.7834090232      0.8338521452
  H6        0.2704473148      3.3309097414      2.5792858946
  H7        1.5126620536     -0.4701482045     -0.3345536365
  C10      -0.2324392502     -0.9787486074     -1.4188954455
  C8        0.1108144953     -1.2091894280      1.0905569998
  C16       0.4435446615     -2.6989470889      0.9774640406
```

```
  H12      -0.9536145665     -1.0997855768      1.2965471047
  N2        0.9363665186      0.7613881271      2.3365852233
  C9        0.8110259309     -0.6157008344      2.3049248570
  C17       1.4719386588      1.3495066011      3.5490732344
  O1        1.2244700189     -1.3159682051      3.1845865060
  C11      -1.4392930901     -2.0864862336     -3.6800748517
  C12       0.5330437839     -1.4137497881     -2.4877189223
  C13      -1.6201576226     -1.1017219113     -1.5030983223
  C14      -2.2179690644     -1.6509076119     -2.6186343550
  C15      -0.0626638857     -1.9643287947     -3.6118289968
  H19       1.6041376217     -1.3271232115     -2.4460389546
  H20      -2.2360263230     -0.7557801883     -0.6930774560
  H21      -3.2877925368     -1.7387789371     -2.6643193114
  H22       0.5491130851     -2.2978165383     -4.4310167547
  H23      -1.9028605764     -2.5145179891     -4.5516882110
  H24       1.5010400703     -2.8384862060      0.7609906527
  H25      -0.1342900999     -3.1594038315      0.1823564211
  H11       0.2258450513     -3.2068361455      1.9106798927
  H2        2.1669291331      2.1388979138      3.2910220231
  H5        1.9784561252      0.5811564826      4.0907951097
  H8        0.6889962057      1.7556553424      4.1682989236

  nuclear repulsion energy.......  1393.662818643 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   4   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.289E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     87     89     89     89     87     85
82
  grid # 2      113     96     96     98     97     97     96
90
  grid # 3      213    184    184    193    183    183    189
175
```

```
  grid # 4      212    327    327    341    327    328    327
311

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     67     90     81     72
68
  grid # 2      118    118    111    106    100     91     79
111
  grid # 3      223    223    206    209    194    173    152
212
  grid # 4      224    223    206    205    339    311    291
208

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       96     81     71    111     89     87     87
89
  grid # 2      105     91     79    123     97     95     95
95
  grid # 3      214    176    140    255    182    182    183
182
  grid # 4      392    293    272    449    326    326    326
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     70     73     73     73     71
71
  grid # 2       96    112    113    118    118    118    109
110
  grid # 3      183    213    212    222    222    224    218
215
  grid # 4      326    212    210    223    224    224    221
215

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       71     71     70     71   2860
  grid # 2      108    111    105    110   3725
  grid # 3      217    216    212    216   7180
  grid # 4      217    212    210    214   9925

  end of program grid


  start of program rwr
  end of program rwr
```

```
  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS     maximum
      e  d  i  u  i                        energy   density    DIIS
      r  t  s  t  d     total energy       change   change     error

etot  1  N  N  2  U  -783.02076627042                 2.8E-04  8.2E-03
etot  2  Y  Y  6  M  -783.03229248937  1.2E-02        1.2E-04  2.0E-03
etot  3  N  Y  2  U  -783.03364015340  1.3E-03        3.2E-05  5.7E-04
etot  4  Y  Y  6  M  -783.03374406665  1.0E-04        1.6E-05  3.4E-04
etot  5  Y  Y  6  M  -783.03376201163  1.8E-05        5.7E-06  1.4E-04
etot  6  Y  Y  6  M  -783.03376594486  3.9E-06        3.8E-06  7.9E-05
etot  7  Y  N  6  M  -783.03376576865 -1.8E-07        0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1393.66281864334
   (E)  Total one-electron terms..... -3831.79219849411
   (I)  Total two-electron terms.....  1655.09561408212
   (L)  Electronic energy............. -2176.69658441199  (E+I)
   (N)  Total energy.................  -783.03376576865  (A+L)

 SCFE: SCF energy: HF    -783.03376576865 hartrees   iterations:
7


 HOMO energy:    -0.30152
 LUMO energy:     0.12782

  Orbital energies:
  -20.52926  -15.60071  -11.34805  -11.28444  -11.25259  -11.25119
  -11.24331  -11.24319  -11.24158  -11.23620  -11.23565  -11.23539
  -11.23386  -11.23329  -11.23293  -11.23271  -11.23215  -11.22674
  -11.20879   -1.39909   -1.26831   -1.16950   -1.14886   -1.10667
   -1.03004   -1.02111   -1.01931   -1.01489   -0.95928   -0.93237
   -0.85937   -0.83628   -0.83166   -0.83027   -0.79032   -0.74283
   -0.71213   -0.69679   -0.68130   -0.66512   -0.64215   -0.63633
   -0.62842   -0.61877   -0.61323   -0.60405   -0.59873   -0.58913
   -0.57006   -0.56091   -0.54946   -0.54153   -0.52949   -0.52012
   -0.51396   -0.50533   -0.49985   -0.49671   -0.48380   -0.47093
   -0.46770   -0.42139   -0.41378   -0.34296   -0.33606   -0.32658
   -0.30152    0.12782    0.13665    0.14220    0.15236    0.20309
    0.23581    0.24231    0.25343    0.26108    0.27459

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	6.352968E-04	-1.889626E-04	1.859963E-03
2	C1	1.377328E-04	-4.012983E-03	-2.658770E-03
3	C2	-4.621400E-04	2.270741E-03	2.158568E-03
4	C3	-8.535699E-04	-1.635754E-04	-3.302643E-03
5	C4	-9.677492E-04	1.421920E-03	-1.568678E-03
6	C5	5.218389E-04	3.428473E-04	2.533169E-03
7	C6	3.773198E-03	-8.479563E-04	2.404846E-03
8	C7	3.812582E-04	-9.145352E-04	-4.105280E-04
9	H3	4.903229E-04	-9.471783E-04	1.203937E-03
10	H4	1.254032E-04	5.264778E-04	3.756103E-04
11	H6	-1.418602E-04	2.501739E-04	-6.599184E-04
12	H7	-4.638474E-04	5.398471E-04	1.814164E-04
13	C10	-1.903113E-03	1.029659E-03	2.330879E-03
14	C8	-7.802332E-04	-6.619837E-04	1.641672E-04
15	C16	-1.520110E-04	-6.927149E-04	-1.430489E-04
16	H12	-4.919678E-04	-1.983353E-04	-2.396040E-04
17	N2	-6.880136E-03	-1.130366E-02	-1.609391E-03
18	C9	1.099385E-03	5.836080E-03	-5.655803E-03
19	C17	3.033194E-03	4.208754E-03	-5.441974E-03
20	O1	2.723844E-04	3.632215E-03	2.915732E-03
21	C11	1.781632E-03	-9.307048E-04	-2.440900E-03
22	C12	1.107748E-03	6.668911E-05	2.525691E-04
23	C13	2.017820E-03	1.265329E-03	2.301579E-03
24	C14	-3.658147E-05	-4.437323E-04	-8.884726E-04
25	C15	-2.447402E-03	-1.129841E-03	-2.358924E-03
26	H19	8.840447E-04	1.402795E-04	1.657628E-04
27	H20	-5.011866E-04	3.354365E-04	8.480332E-04
28	H21	-1.241199E-03	1.119685E-05	1.124635E-04
29	H22	2.970430E-04	-1.184714E-04	-3.132704E-04
30	H23	1.205196E-04	-1.620186E-05	8.859471E-05
31	H24	-1.956572E-03	-2.037392E-04	3.406483E-04
32	H25	1.225083E-03	1.026667E-03	1.402165E-03
33	H11	7.420147E-04	1.523856E-03	-2.403144E-03
34	H2	4.153655E-04	3.855323E-04	9.452504E-04
35	H5	3.653025E-03	-3.597237E-03	3.395932E-03
36	H8	-3.891349E-03	2.284840E-03	3.765373E-03
total		-4.566080E-04	7.267322E-04	-3.484093E-04

```
 end of program der1b
```

```
  start of program geopt   5

  geometry optimization step  5
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:           6.0333E-05 .  (  5.0000E-05 )
  gradient maximum:        1.0034E-02 .  (  4.5000E-04 )
  gradient rms:            2.1000E-03 .  (  3.0000E-04 )
  step size:   0.17732  trust radius:   0.30000
  displacement maximum:    7.8977E-02 .  (  1.8000E-03 )
  displacement rms:        1.6054E-02 .  (  1.2000E-03 )
  predicted energy change:    -6.8401E-04    geom step:   1.7732E-
01    full step:   1.7732E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.1450E-02     y:     1.0749E-03     z:     4.6143E-03

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -0.4730932560     1.5350165766    -1.9158290603
  C1       -0.3275788293     1.9202065735    -0.9247678798
  C2        0.0543319924     2.9157761918     1.6106075534
  C3        0.1251553697     1.0652890804     0.0653554294
  C4       -0.5914684395     3.2570810448    -0.6692721484
  C5       -0.4067538414     3.7484857155     0.6044012401
  C6        0.3357851171     1.5796445807     1.3477511057
  C7        0.4502828387    -0.3981066979    -0.1884948402
  H3       -0.9386669555     3.8985984908    -1.4586922504
  H4       -0.6153448756     4.7809782350     0.8284326578
  H6        0.1923630363     3.3178388164     2.5956232074
  H7        1.5278289061    -0.4677096856    -0.3504033084
  C10      -0.2322276233    -0.9749156270    -1.4184666642
  C8        0.1330303509    -1.2221121495     1.0762712301
  C16       0.5116466057    -2.6963499432     0.9540034854
  H12      -0.9375953617    -1.1467043574     1.2668584746
  N2        0.8744729145     0.7519777261     2.3569870427
  C9        0.8003008563    -0.6146497365     2.3032178734
  C17       1.4470526069     1.3503032253     3.5548757175
  O1        1.2256186175    -1.2956256324     3.1957796594
  C11      -1.4687277699    -2.0864590094    -3.6695950566
  C12       0.5201354851    -1.4410568514    -2.4866410270
  C13      -1.6211810237    -1.0683464146    -1.4973340029
  C14      -2.2335827202    -1.6196482610    -2.6083679951
```

```
  C15      -0.0909871934     -1.9931471858     -3.6058524109
  H19       1.5945974571     -1.3789666746     -2.4483991559
  H20      -2.2289642325     -0.7000824047     -0.6878915776
  H21      -3.3076305048     -1.6841393753     -2.6485656306
  H22       0.5131845628     -2.3499468974     -4.4226590953
  H23      -1.9457108667     -2.5154181629     -4.5343780038
  H24       1.5716217012     -2.8053008675      0.7503882864
  H25      -0.0387417979     -3.1643301485      0.1483982341
  H11       0.3006114500     -3.2188743651      1.8759625767
  H2        2.1198286508      2.1524761534      3.2805029773
  H5        1.9905818991      0.5893507757      4.0839702166
  H8        0.6781150609      1.7433694196      4.2088162262

  nuclear repulsion energy.......  1394.194196772 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   5   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.280E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     86     89     88     89     87     84
82
  grid # 2      113     96     96     98     97     97     95
90
  grid # 3      213    184    183    192    182    183    189
175
  grid # 4      213    327    328    338    327    328    326
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     67     90     83     73
68
  grid # 2      118    118    112    106    100     91     80
111
```

```
  grid # 3      223    223    207    209    192    176    148
213
  grid # 4      224    223    207    203    337    309    286
209

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       96     81     69    111     89     87     87
89
  grid # 2      104     92     79    122     97     95     95
95
  grid # 3      211    176    145    255    181    182    183
183
  grid # 4      391    293    274    449    326    326    326
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     71     73     73     73     71
71
  grid # 2       96    111    113    118    118    118    108
110
  grid # 3      182    213    212    223    223    224    218
215
  grid # 4      326    213    209    223    224    224    218
212

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       70     71     70     71   2858
  grid # 2      108    111    106    110   3724
  grid # 3      218    216    212    216   7180
  grid # 4      214    213    209    215   9908

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                    energy  density   DIIS
      r  t  s  t  d     total energy   change  change    error

etot  1  N  N  2  U  -783.02750102839           1.9E-04  6.0E-03
etot  2  Y  Y  6  M  -783.03345176139  6.0E-03   8.3E-05  2.2E-03
```

```
etot   3  N  Y  2  U  -783.03421229436  7.6E-04  2.4E-05  5.6E-04
etot   4  Y  Y  6  M  -783.03425171005  3.9E-05  1.2E-05  2.6E-04
etot   5  Y  Y  6  M  -783.03426675380  1.5E-05  4.2E-06  8.1E-05
etot   6  Y  N  6  M  -783.03426604715 -7.1E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1394.19419677164
   (E)  Total one-electron terms..... -3832.86176139766
   (I)  Total two-electron terms.....  1655.63329857887
   (L)  Electronic energy..... -2177.22846281879  (E+I)
   (N)  Total energy.............  -783.03426604715  (A+L)

 SCFE: SCF energy: HF    -783.03426604715 hartrees   iterations:
6


 HOMO energy:    -0.30086
 LUMO energy:     0.12726

  Orbital energies:
  -20.52569  -15.60040  -11.34599  -11.28463  -11.25396  -11.25140
  -11.24376  -11.24353  -11.24126  -11.23667  -11.23630  -11.23621
  -11.23405  -11.23381  -11.23357  -11.23354  -11.23223  -11.22664
  -11.20764   -1.39696   -1.26844   -1.16951   -1.14874   -1.10737
   -1.03115   -1.02062   -1.01842   -1.01502   -0.96030   -0.93307
   -0.85937   -0.83861   -0.83170   -0.83009   -0.79021   -0.74311
   -0.71249   -0.69635   -0.68098   -0.66511   -0.64158   -0.63626
   -0.62870   -0.61777   -0.61248   -0.60426   -0.59881   -0.58805
   -0.57028   -0.56129   -0.54879   -0.54063   -0.52916   -0.52066
   -0.51449   -0.50558   -0.49997   -0.49661   -0.48390   -0.47084
   -0.46838   -0.42066   -0.41263   -0.34339   -0.33608   -0.32659
   -0.30086    0.12726    0.13637    0.14155    0.15174    0.20458
    0.23573    0.24178    0.25271    0.26189    0.27471

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
```

1	H1	-3.816687E-04	9.176652E-05	-5.209111E-04
2	C1	-4.387183E-04	2.911026E-05	-1.166443E-03
3	C2	4.664693E-04	8.543396E-05	1.487278E-03
4	C3	-7.310630E-04	3.704576E-04	-1.843909E-04
5	C4	-5.561690E-04	-1.030513E-04	-2.391189E-03
6	C5	2.271547E-04	1.243283E-03	1.979541E-03
7	C6	1.396023E-03	9.523323E-04	1.911361E-03
8	C7	1.985156E-03	-5.739051E-04	2.411974E-04
9	H3	-1.880618E-04	-5.322325E-05	-4.299891E-04
10	H4	8.022218E-05	-8.167765E-04	-1.446346E-04
11	H6	1.003403E-04	-4.913884E-04	-2.237230E-04
12	H7	-1.168444E-03	-1.825105E-04	2.017480E-05
13	C10	2.105611E-04	-4.060455E-04	-1.034686E-03
14	C8	-2.377387E-04	7.518305E-04	1.473918E-03
15	C16	-1.038249E-04	-5.617158E-04	1.363690E-05
16	H12	3.365015E-05	1.666225E-05	9.739531E-06
17	N2	-1.034658E-03	9.756522E-04	-2.811521E-04
18	C9	1.422291E-03	-4.468535E-04	1.351534E-03
19	C17	8.001469E-04	4.082844E-04	-7.382558E-04
20	O1	-1.407451E-03	-1.164586E-03	-1.703011E-03
21	C11	-4.800767E-04	-7.375261E-05	-3.246766E-04
22	C12	3.266542E-04	-2.254225E-04	-5.817589E-04
23	C13	-9.659120E-04	-1.051850E-04	1.827135E-04
24	C14	-2.573035E-04	1.423362E-04	3.598998E-04
25	C15	5.329591E-04	-1.163979E-04	-3.226177E-04
26	H19	-2.657218E-04	1.244054E-04	7.701009E-05
27	H20	3.652363E-04	-2.042697E-04	-7.531744E-04
28	H21	5.024247E-04	6.073941E-05	5.217940E-05
29	H22	-2.060279E-04	2.515308E-04	5.362930E-04
30	H23	3.263884E-04	2.899916E-04	6.034378E-04
31	H24	6.741604E-04	8.124307E-05	-1.654580E-04
32	H25	-3.649737E-04	-9.768345E-05	-1.094634E-04
33	H11	-2.388963E-04	1.536885E-04	1.726793E-04
34	H2	-2.194149E-05	4.522229E-04	-7.103327E-04
35	H5	6.185348E-04	-5.346366E-04	1.621277E-04
36	H8	-1.389617E-03	5.333895E-04	8.172180E-04
total		-3.698949E-04	8.569570E-04	-3.339279E-04

```
 end of program der1b


 start of program geopt   6

 geometry optimization step  6
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:          -5.0028E-04 .  (  5.0000E-05 )
```

```
  gradient maximum:        5.0487E-03 .  (  4.5000E-04 )
  gradient rms:            8.9609E-04 .  (  3.0000E-04 )
  step size:   0.13770  trust radius:   0.30000
  displacement maximum:    6.1744E-02 .  (  1.8000E-03 )
  displacement rms:        1.2466E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.5527E-04    geom step:   1.3770E-
01    full step:   1.3770E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.3094E-03     y:    -3.9766E-04     z:     8.6490E-05

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -0.5726813221      1.5273415377     -1.8931618699
  C1       -0.3877292369      1.9172407008     -0.9099391904
  C2        0.0868323850      2.9268239424      1.6187605825
  C3        0.1034562262      1.0703935793      0.0711203042
  C4       -0.6417524127      3.2554349013     -0.6487165941
  C5       -0.4060547481      3.7534006939      0.6214109841
  C6        0.3529824582      1.5890380486      1.3510574069
  C7        0.4317703649     -0.3955417113     -0.1795800607
  H3       -1.0199664301      3.8929219966     -1.4280340873
  H4       -0.6056632177      4.7859731586      0.8463846212
  H6        0.2556999921      3.3286095367      2.5982808615
  H7        1.5086379438     -0.4682759844     -0.3263482400
  C10      -0.2278709659     -0.9776669354     -1.4218229960
  C8        0.0950592511     -1.2059762465      1.0902768807
  C16       0.4296547579     -2.6949491268      0.9725782660
  H12      -0.9724980129     -1.0973057476      1.2855437076
  N2        0.8926096338      0.7579426353      2.3551844043
  C9        0.7917201930     -0.6098541397      2.3065164785
  C17       1.5131880732      1.3515918122      3.5279600896
  O1        1.2084267792     -1.3041443126      3.1935555354
  C11      -1.4175274396     -2.1009616596     -3.6928249934
  C12       0.5458714913     -1.4213029579     -2.4857177450
  C13      -1.6147883302     -1.0971791512     -1.5164176278
  C14      -2.2034819731     -1.6545978239     -2.6370503111
  C15      -0.0418310656     -1.9800311941     -3.6146052271
  H19       1.6176755938     -1.3334176291     -2.4331840317
  H20      -2.2382460261     -0.7440489158     -0.7144103176
  H21      -3.2747867212     -1.7403771932     -2.6895132100
  H22       0.5782446520     -2.3191312492     -4.4252366082
  H23      -1.8765816043     -2.5354658104     -4.5630432881
  H24       1.4856396907     -2.8351650387      0.7586615796
  H25      -0.1451012315     -3.1510936573      0.1765341785
  H11       0.2104402576     -3.2024206528      1.9008850173
  H2        2.1552144309      2.1707454357      3.2342941050
  H5        2.0994089356      0.5927040067      4.0160963549
  H8        0.7673732619      1.7208228849      4.2254504811
```

```
  nuclear repulsion energy.......  1393.055123690 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   6   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.355E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     89     86
82
  grid # 2      113     96     96     98     97     97     93
90
  grid # 3      213    184    184    192    184    184    189
175
  grid # 4      213    327    328    341    327    328    327
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     66     91     82     74
68
  grid # 2      118    118    112    106    100     90     80
111
  grid # 3      223    223    207    209    193    173    148
213
  grid # 4      224    223    205    205    337    312    287
208

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       94     81     69    111     89     87     87
89
  grid # 2      105     92     80    123     97     95     95
95
```

```
  grid # 3      212    176    144    257    182    183    183
183
  grid # 4      391    293    274    450    326    326    326
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     70     73     73     73     71
71
  grid # 2       96    113    113    118    118    118    109
110
  grid # 3      182    213    212    223    223    224    218
215
  grid # 4      326    213    211    223    224    224    218
212

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       71     71     70     71   2862
  grid # 2      108    111    108    111   3730
  grid # 3      217    215    212    217   7185
  grid # 4      214    213    209    218   9921

  end of program grid


  start of program rwr
 recomputing RwR matrix  17    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g                                                 RMS    maximum
       t  p  i  c  r                                     energy  density   DIIS
       e  d  i  u  i                    total energy     change  change    error

etot   1  N  N  2  U  -783.02884572067                          1.6E-04  4.4E-03
etot   2  Y  Y  6  M  -783.03370737433  4.9E-03  7.3E-05  1.8E-03
etot   3  Y  Y  6  M  -783.03431816575  6.1E-04  2.0E-05  4.0E-04
etot   4  N  Y  2  U  -783.03433585814  1.8E-05  8.5E-06  1.7E-04
etot   5  Y  Y  6  M  -783.03434373753  7.9E-06  3.4E-06  5.0E-05
etot   6  Y  N  6  M  -783.03434508372  1.3E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1393.05512369041
   (E)  Total one-electron terms..... -3830.58777047841
   (I)  Total two-electron terms.....  1654.49830170429
   (L)  Electronic energy..... -2176.08946877413  (E+I)
```

```
   (N)  Total energy.................  -783.03434508372  (A+L)

 SCFE: SCF energy: HF    -783.03434508372 hartrees   iterations:
6


 HOMO energy:    -0.30011
 LUMO energy:     0.12684

  Orbital energies:
 -20.52660  -15.60092  -11.34666  -11.28514  -11.25510  -11.25132
 -11.24412  -11.24354  -11.24226  -11.23701  -11.23672  -11.23629
 -11.23421  -11.23419  -11.23391  -11.23361  -11.23260  -11.22762
 -11.20767   -1.39659   -1.26924   -1.16870   -1.14755   -1.10644
  -1.02997   -1.01965   -1.01825   -1.01536   -0.96019   -0.93260
  -0.85917   -0.83804   -0.83173   -0.82968   -0.78983   -0.74334
  -0.71209   -0.69639   -0.68070   -0.66473   -0.64188   -0.63662
  -0.62749   -0.61841   -0.61186   -0.60433   -0.59983   -0.58838
  -0.57026   -0.56086   -0.54933   -0.53996   -0.52863   -0.52093
  -0.51455   -0.50485   -0.49959   -0.49676   -0.48389   -0.47000
  -0.46811   -0.42047   -0.41278   -0.34305   -0.33561   -0.32730
  -0.30011    0.12684    0.13635    0.14139    0.15122    0.20356
   0.23580    0.24196    0.25320    0.26161    0.27452

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
recomputing RwR matrix  17    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
   1     H1      2.271081E-04   1.216095E-04   1.082944E-04
   2     C1      5.186854E-04   2.806669E-04   1.469776E-03
   3     C2     -4.665463E-04  -5.998461E-04  -1.766580E-03
   4     C3      9.534496E-04   4.456467E-04   1.967966E-03
   5     C4      4.935329E-04   1.305581E-03   3.145803E-03
   6     C5     -5.599219E-04  -8.946850E-04  -3.210444E-03
   7     C6     -1.657815E-03  -6.058748E-04  -2.566135E-03
   8     C7     -1.163267E-03   1.312031E-04   1.680837E-04
   9     H3      4.316664E-05   1.129883E-04   4.280720E-04
  10     H4     -1.173277E-04   3.166913E-04  -9.211525E-05
```

```
  11    H6     -1.798394E-04   2.532126E-04   4.970073E-05
  12    H7      5.832312E-04   1.548604E-04   2.583969E-04
  13    C10    -3.775088E-04   2.025095E-05  -3.476817E-04
  14    C8      2.314555E-04  -9.789165E-04  -8.489841E-04
  15    C16     1.453268E-05   1.483674E-03   2.893736E-04
  16    H12     5.733456E-04  -7.991196E-05   5.433509E-05
  17    N2      1.142071E-03  -2.562852E-03  -2.833270E-03
  18    C9     -3.073795E-04  -1.134186E-03   1.979257E-03
  19    C17    -8.705439E-05  -6.225941E-04   2.277256E-03
  20    O1     -4.792424E-04   2.644846E-03  -1.674648E-03
  21    C11     2.120048E-04   4.169085E-04   9.639898E-04
  22    C12    -7.400468E-04   2.009130E-04   6.220562E-04
  23    C13     6.874647E-04  -3.551548E-04  -1.012763E-03
  24    C14     7.270571E-04  -7.349147E-05  -2.745324E-04
  25    C15    -4.743025E-04   5.516508E-04   9.612754E-04
  26    H19    -4.947400E-05  -2.425096E-04  -2.741908E-04
  27    H20    -2.278509E-04   2.198601E-05   3.444204E-04
  28    H21    -4.668025E-05   3.508883E-05  -3.332067E-05
  29    H22     1.964218E-04  -1.206227E-04  -3.175738E-04
  30    H23    -2.521789E-05  -3.636574E-05  -1.672455E-04
  31    H24    -6.567914E-04  -5.380175E-05   6.579315E-05
  32    H25     1.616368E-04   1.794365E-04   9.641891E-05
  33    H11     1.582532E-04  -1.572193E-04   1.874749E-04
  34    H2      2.570725E-04   4.053167E-04  -1.199306E-03
  35    H5     -1.219002E-04   1.821590E-04   6.048539E-04
  36    H8      3.284274E-04  -1.003100E-04   3.568440E-04
 -----------   -------------  -------------  -------------
    total      -2.292502E-04   6.463486E-04  -2.193489E-04

  end of program der1b


  start of program geopt   7

  geometry optimization step  7
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -7.9037E-05 .  (  5.0000E-05 )
  gradient maximum:        4.6013E-03 .  (  4.5000E-04 )
  gradient rms:            8.8095E-04 .  (  3.0000E-04 )
  step size:   0.06047  trust radius:   0.30000
  displacement maximum:    3.4926E-02 .  (  1.8000E-03 )
  displacement rms:        5.4749E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.1554E-04    geom step:   6.0472E-
02    full step:   6.0472E-02
  molecular structure not yet converged...
```

```
 center of mass moved by:
    x:     3.4406E-04     y:    -4.5979E-04     z:     3.2713E-04

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -0.5699917377     1.5301542015    -1.8905411925
 C1       -0.3904661091     1.9174633877    -0.9058012081
 C2        0.0722912184     2.9199926793     1.6192544872
 C3        0.1018150237     1.0685880080     0.0720184482
 C4       -0.6534282111     3.2538162091    -0.6429268828
 C5       -0.4260344983     3.7482515384     0.6250615819
 C6        0.3491246356     1.5853896009     1.3493857014
 C7        0.4301905337    -0.3971696002    -0.1763189920
 H3       -1.0330556950     3.8916721814    -1.4209841494
 H4       -0.6347004231     4.7784419952     0.8530599405
 H6        0.2376062138     3.3192942317     2.5998557534
 H7        1.5085562443    -0.4705726901    -0.3174073551
 C10      -0.2255021351    -0.9786199821    -1.4201846265
 C8        0.0891493383    -1.2057173752     1.0939397723
 C16       0.4140300438    -2.6967891183     0.9798455136
 H12      -0.9778020152    -1.0896264356     1.2910669329
 N2        0.9085882864     0.7552661779     2.3460140307
 C9        0.7922540602    -0.6102335659     2.3069935904
 C17       1.5363340714     1.3527810435     3.5138086691
 O1        1.2082567921    -1.3001526255     3.1952935765
 C11      -1.4078398149    -2.0922215504    -3.6966800535
 C12       0.5517002469    -1.4279764966    -2.4777865557
 C13      -1.6121923432    -1.0907832806    -1.5227388085
 C14      -2.1975318691    -1.6426780030    -2.6462747177
 C15      -0.0324528324    -1.9813120801    -3.6095465179
 H19       1.6237006138    -1.3498167715    -2.4197930486
 H20      -2.2379843655    -0.7350894280    -0.7231078319
 H21      -3.2688614471    -1.7209477216    -2.7055790072
 H22       0.5903534551    -2.3248943979    -4.4168227515
 H23      -1.8636381710    -2.5219175566    -4.5711693736
 H24       1.4671489178    -2.8448072509     0.7543388598
 H25      -0.1719581135    -3.1551496701     0.1917542186
 H11       0.2016967811    -3.1985875984     1.9142761709
 H2        2.1725424562     2.1726568093     3.2038223330
 H5        2.1302164122     0.5994436776     4.0021428942
 H8        0.7946754746     1.7226884890     4.2164439812

 nuclear repulsion energy.......  1393.679119978 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   7   /
------------------------------------------------

 end of program geopt
```

```
  start of program onee
  smallest eigenvalue of S:    3.316E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
82
  grid # 2      113     96     96     98     97     97     93
90
  grid # 3      213    184    184    192    183    183    195
175
  grid # 4      212    327    328    339    327    328    329
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     66     90     82     73
68
  grid # 2      118    118    112    106    100     90     80
110
  grid # 3      223    223    207    209    192    174    146
213
  grid # 4      224    223    207    206    337    310    285
208

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       94     81     71    111     89     87     87
89
  grid # 2      105     92     79    123     97     95     95
95
  grid # 3      211    176    142    257    182    182    183
183
  grid # 4      391    292    273    450    326    326    326
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
```

```
  grid # 1       89     73     70     73     73     73     71
71
  grid # 2       96    113    113    118    118    118    109
110
  grid # 3      182    213    212    223    223    224    218
215
  grid # 4      326    213    211    223    224    224    218
214

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       71     71     70     71   2860
  grid # 2      108    111    108    111   3728
  grid # 3      217    215    212    217   7183
  grid # 4      214    212    209    218   9918

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  1  U  -783.03374900811            7.7E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03425399363  5.0E-04  2.5E-05  5.2E-04
etot  3  Y  Y  4  M  -783.03431710245  6.3E-05  6.9E-06  1.3E-04
etot  4  Y  Y  4  M  -783.03432047845  3.4E-06  3.4E-06  5.6E-05
etot  5  Y  N  4  M  -783.03432189558  1.4E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1393.67911997751
   (E)  Total one-electron terms..... -3831.84105412155
   (I)  Total two-electron terms.....  1655.12761224846
   (L)  Electronic energy............. -2176.71344187310  (E+I)
   (N)  Total energy.................  -783.03432189558  (A+L)

 SCFE: SCF energy: HF    -783.03432189558 hartrees   iterations:
5


 HOMO energy:    -0.30109
 LUMO energy:     0.12735

  Orbital energies:
```

```
 -20.52621  -15.60029  -11.34593  -11.28451  -11.25545  -11.25120
 -11.24371  -11.24351  -11.24183  -11.23658  -11.23640  -11.23591
 -11.23388  -11.23387  -11.23354  -11.23328  -11.23246  -11.22724
 -11.20812   -1.39749   -1.26893   -1.16906   -1.14828   -1.10662
  -1.03005   -1.02020   -1.01868   -1.01515   -0.96000   -0.93259
  -0.85892   -0.83792   -0.83174   -0.82996   -0.78990   -0.74326
  -0.71199   -0.69632   -0.68102   -0.66496   -0.64183   -0.63631
  -0.62783   -0.61837   -0.61221   -0.60428   -0.59881   -0.58849
  -0.57028   -0.56075   -0.54938   -0.54015   -0.52869   -0.52085
  -0.51436   -0.50494   -0.49989   -0.49661   -0.48376   -0.47034
  -0.46809   -0.42019   -0.41263   -0.34306   -0.33571   -0.32707
  -0.30109    0.12735    0.13675    0.14170    0.15157    0.20407
   0.23568    0.24202    0.25327    0.26126    0.27470

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  17    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
   1     H1     -8.756323E-07  -5.549027E-05  -3.027852E-04
   2     C1      3.460237E-05  -3.815773E-04   4.978475E-06
   3     C2     -2.730008E-04  -7.685054E-05  -5.589996E-04
   4     C3      2.889074E-04   4.057053E-06   1.782790E-04
   5     C4     -3.778517E-05  -2.701043E-05  -2.247732E-05
   6     C5      2.333149E-04  -2.097944E-04   5.299008E-04
   7     C6      2.513904E-04   1.629590E-04   8.878774E-06
   8     C7     -4.181213E-04  -1.309624E-04  -9.886016E-05
   9     H3     -8.508096E-06  -1.192945E-04   4.262361E-05
  10     H4      6.281730E-05   2.009668E-04   1.699253E-04
  11     H6      4.346850E-05   4.586833E-04   5.003538E-04
  12     H7      1.264357E-05   1.216860E-04   8.291130E-05
  13     C10    -2.591912E-04   1.126998E-04   2.923811E-04
  14     C8     -4.297350E-04  -5.688182E-04  -3.393951E-04
  15     C16    -8.309263E-05   5.594376E-04   1.818946E-04
  16     H12     8.389005E-04  -1.880512E-04  -1.233930E-04
  17     N2     -9.111789E-04  -5.544360E-04  -2.683171E-03
  18     C9     -3.770045E-04  -6.003563E-05  -5.139534E-05
  19     C17     2.303698E-04   4.991149E-04   1.053068E-03
  20     O1      3.328331E-04  -4.186373E-05   6.468095E-04
```

```
 21    C11    -1.421224E-05  -7.206171E-05  -1.681081E-04
 22    C12     6.846973E-05   2.643001E-04   5.150298E-04
 23    C13     6.058929E-04   3.071575E-04   4.294553E-04
 24    C14     6.931099E-05  -2.456700E-04  -5.552205E-04
 25    C15    -3.142517E-04  -1.306566E-04  -3.112255E-04
 26    H19     1.228372E-04   3.240965E-05  -4.198892E-05
 27    H20    -5.996181E-05  -3.347475E-06   1.025972E-04
 28    H21    -1.604856E-04  -4.716251E-05  -3.304380E-05
 29    H22    -1.360587E-05   1.056759E-05  -5.820001E-05
 30    H23    -2.923334E-05  -3.476214E-05  -4.039000E-05
 31    H24    -1.022132E-03   4.082317E-05   2.813084E-04
 32    H25     5.203043E-04   6.255197E-04   6.463181E-04
 33    H11     3.534913E-04   2.579826E-04  -6.379859E-04
 34    H2     -3.870477E-04  -1.930727E-04   1.454670E-04
 35    H5     -2.683275E-04   1.447454E-04   2.148347E-05
 36    H8      8.164214E-04  -8.398156E-05  -1.348185E-05
-----------   -------------  -------------  -------------
   total      -1.817755E-04   5.782108E-04  -2.064574E-04

 end of program der1b


 start of program geopt   8

 geometry optimization step  8
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:           2.3188E-05 *  (  5.0000E-05 )
 gradient maximum:        1.4547E-03 .  (  4.5000E-04 )
 gradient rms:            4.1313E-04 .  (  3.0000E-04 )
 step size:   0.14222  trust radius:   0.30000
 displacement maximum:    7.7289E-02 .  (  1.8000E-03 )
 displacement rms:        1.2876E-02 .  (  1.2000E-03 )
 predicted energy change:    -7.6457E-05    geom step:   1.4222E-
01    full step:   1.4222E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:    -1.1837E-02     y:     1.5469E-03     z:     1.7140E-03

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -0.5864987654     1.5324898101    -1.8892765297
 C1       -0.3956998422     1.9195562430    -0.9056281219
 C2        0.0957942140     2.9237885776     1.6136613176
 C3        0.1025973714     1.0702500403     0.0678206425
 C4       -0.6504765272     3.2573494231    -0.6407979608
```

```
 C5       -0.4069361401      3.7535624101      0.6236165469
 C6        0.3620731334      1.5879999742      1.3414037802
 C7        0.4274283216     -0.3960101603     -0.1776989750
 H3       -1.0367199390      3.8947947483     -1.4156452034
 H4       -0.6057910084      4.7854300530      0.8534501851
 H6        0.2740789874      3.3250590621      2.5928754071
 H7        1.5060525124     -0.4675239688     -0.3171219588
 C10      -0.2266746243     -0.9787766880     -1.4216675261
 C8        0.0896716612     -1.2085060093      1.0905559375
 C16       0.4473539462     -2.6860738676      0.9832255305
 H12      -0.9760544377     -1.1152952934      1.2744031729
 N2        0.9259650237      0.7537619706      2.3277745596
 C9        0.7621697719     -0.6092625771      2.3155703929
 C17       1.5470848239      1.3389197170      3.5093837004
 O1        1.1222606524     -1.2963838725      3.2329542278
 C11      -1.4031923589     -2.0976607713     -3.6992472965
 C12       0.5525077750     -1.4265411131     -2.4786716594
 C13      -1.6125455336     -1.0949136988     -1.5258181170
 C14      -2.1950077187     -1.6496893230     -2.6496126004
 C15      -0.0286756405     -1.9818689463     -3.6108369694
 H19       1.6240440490     -1.3454729980     -2.4209657149
 H20      -2.2405092741     -0.7412966926     -0.7271393056
 H21      -3.2658783776     -1.7317552747     -2.7097592412
 H22       0.5957648198     -2.3235540528     -4.4174109945
 H23      -1.8568860631     -2.5296352110     -4.5735918276
 H24       1.5010050846     -2.8119731186      0.7814416001
 H25      -0.1078593304     -3.1477020220      0.1847805523
 H11       0.2333637741     -3.1974560065      1.9072578535
 H2        2.1928150888      2.1540692087      3.2018155473
 H5        2.1294412902      0.5774573997      4.0017525878
 H8        0.8062274999      1.7142304430      4.2092071965

 nuclear repulsion energy.......  1393.881595876 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   8   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.309E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe


 start of program grid
```

number of gridpoints:

atom	H1	C1	C2	C3	C4	C5	C6	C7
grid # 1	71	88	89	88	89	87	86	82
grid # 2	113	96	96	98	97	97	93	90
grid # 3	213	184	183	192	183	183	191	175
grid # 4	212	327	328	339	327	328	326	311

number of gridpoints:

atom	H3	H4	H6	H7	C10	C8	C16	H12
grid # 1	73	73	70	68	90	82	71	68
grid # 2	118	118	112	106	100	91	79	110
grid # 3	223	223	207	209	192	176	153	213
grid # 4	224	223	207	206	337	309	289	204

number of gridpoints:

atom	N2	C9	C17	O1	C11	C12	C13	C14
grid # 1	95	81	70	111	89	87	87	89
grid # 2	105	93	79	123	97	95	95	95
grid # 3	214	176	143	257	181	182	183	183
grid # 4	393	292	272	450	326	326	326	326

number of gridpoints:

atom	C15	H19	H20	H21	H22	H23	H24	H25
grid # 1	89	73	71	73	73	73	71	70
grid # 2	96	113	113	118	118	118	109	108
grid # 3	182	213	212	223	223	224	217	214
grid # 4	326	212	211	223	224	224	216	211

number of gridpoints:

atom	H11	H2	H5	H8	total
grid # 1	70	71	70	71	2859
grid # 2	108	111	107	110	3725

```
  grid # 3      217    215    213    217   7189
  grid # 4      214    214    209    218   9910

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                          RMS    maximum
      e  d  i  u  i                          energy  density   DIIS
      r  t  s  t  d     total energy         change  change    error

etot  1  N  N  2  U  -783.03069846597                 2.3E-04  4.4E-03
etot  2  Y  Y  6  M  -783.03389217665  3.2E-03  6.3E-05  1.8E-03
etot  3  Y  Y  6  M  -783.03425958179  3.7E-04  1.4E-05  4.0E-04
etot  4  N  Y  2  U  -783.03427925014  2.0E-05  9.6E-06  2.2E-04
etot  5  Y  Y  6  M  -783.03428689346  7.6E-06  3.6E-06  7.5E-05
etot  6  Y  N  6  M  -783.03428901507  2.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1393.88159587636
   (E)  Total one-electron terms..... -3832.22643817311
   (I)  Total two-electron terms.....  1655.31055328169
   (L)  Electronic energy............. -2176.91588489143  (E+I)
   (N)  Total energy.................  -783.03428901507  (A+L)

 SCFE: SCF energy: HF    -783.03428901507 hartrees   iterations:
6


 HOMO energy:    -0.30108
 LUMO energy:     0.12752

  Orbital energies:
  -20.52677  -15.60066  -11.34631  -11.28442  -11.25577  -11.25099
  -11.24383  -11.24213  -11.24154  -11.23652  -11.23650  -11.23592
  -11.23394  -11.23392  -11.23364  -11.23340  -11.23255  -11.22712
  -11.20563   -1.39651   -1.26916   -1.16920   -1.14836   -1.10742
   -1.03151   -1.02039   -1.01885   -1.01522   -0.95951   -0.93346
   -0.86016   -0.83822   -0.83193   -0.83019   -0.79011   -0.74376
   -0.71253   -0.69669   -0.68088   -0.66525   -0.64201   -0.63592
   -0.62802   -0.61897   -0.61271   -0.60469   -0.59732   -0.58855
   -0.57055   -0.56095   -0.55007   -0.54078   -0.52892   -0.52079
   -0.51477   -0.50572   -0.50015   -0.49663   -0.48353   -0.47109
   -0.46850   -0.42067   -0.41301   -0.34313   -0.33572   -0.32751
   -0.30108    0.12752    0.13681    0.14163    0.15178    0.20285
```

```
   0.23559    0.24212    0.25353    0.26162    0.27507

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  17    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	6.330900E-05	1.599930E-04	2.515359E-04
2	C1	-3.820982E-04	-4.285491E-04	-8.349071E-04
3	C2	1.602821E-04	4.899909E-04	7.304304E-04
4	C3	-3.587286E-04	-3.341458E-05	2.212094E-04
5	C4	-1.102049E-04	1.653245E-04	-1.997025E-04
6	C5	3.161384E-05	-2.058403E-04	2.464008E-04
7	C6	6.445727E-04	4.737891E-04	-7.510266E-04
8	C7	5.880822E-04	-1.997425E-04	-2.750985E-04
9	H3	3.917162E-05	8.936848E-05	-9.213597E-05
10	H4	-1.090950E-04	1.209701E-04	-1.142084E-04
11	H6	-9.445179E-05	-1.923460E-04	-4.825334E-04
12	H7	1.231873E-04	-4.133004E-06	-1.204272E-04
13	C10	2.001550E-04	6.262828E-06	1.235108E-04
14	C8	1.388942E-03	1.619742E-03	-1.060896E-04
15	C16	-6.879629E-04	3.757640E-04	6.441790E-04
16	H12	-3.141873E-03	7.106869E-05	5.415809E-04
17	N2	5.052635E-04	-3.958456E-03	4.994791E-03
18	C9	8.846687E-04	2.243870E-04	1.490423E-03
19	C17	1.134149E-03	1.583455E-03	-1.534303E-03
20	O1	-4.518351E-04	3.329679E-03	-2.459230E-03
21	C11	-4.672105E-04	7.815982E-05	1.268888E-04
22	C12	3.969949E-05	2.935703E-04	3.232656E-04
23	C13	3.717642E-04	1.275869E-04	4.275834E-04
24	C14	1.326799E-04	-3.021929E-04	-7.038506E-04
25	C15	-1.015598E-04	-1.449456E-04	-2.459885E-04
26	H19	3.216642E-04	8.663778E-05	1.294132E-04
27	H20	-1.293120E-04	8.581572E-05	1.848546E-04
28	H21	-2.716379E-04	-1.616202E-05	-1.584307E-05
29	H22	1.299565E-04	-4.475512E-05	-1.362686E-04
30	H23	-7.439133E-05	-4.153185E-05	-1.040075E-04
31	H24	4.100479E-03	-1.341698E-04	-1.170002E-03
32	H25	-2.250899E-03	-2.461442E-03	-2.986923E-03

```
  33    H11    -1.308167E-03  -5.745324E-04   1.900844E-03
  34    H2     -6.615611E-04  -8.134757E-04   1.238995E-03
  35    H5     -6.004191E-04   8.378899E-04  -9.494906E-04
  36    H8      9.883114E-05  -6.928102E-05  -2.187820E-04
 -----------   -------------  -------------  -------------
    total      -2.429366E-04   5.944840E-04   7.508651E-05

  end of program der1b


  start of program geopt   9

  geometry optimization step  9
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  ** restarting optimization from step    8 **


  energy change:           3.2881E-05 *  (  5.0000E-05 )
  gradient maximum:        1.4547E-03 .  (  4.5000E-04 )
  gradient rms:            4.1313E-04 .  (  3.0000E-04 )
  step size:   0.06128  trust radius:   0.30000
  displacement maximum:    2.6088E-02 .  (  1.8000E-03 )
  displacement rms:        5.5477E-03 .  (  1.2000E-03 )
  predicted energy change:    -4.8038E-05    geom step:   6.1277E-
02    full step:   6.1277E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     2.7756E-17     y:    -1.2490E-16     z:    -2.2204E-16

  new geometry:
                                 angstroms
  atom            x                y                z
  H1       -0.6028821114     1.5255573902    -1.8836524125
  C1       -0.4096792489     1.9141786601    -0.9006449053
  C2        0.0878492783     2.9236296067     1.6172113089
  C3        0.0927510258     1.0681321060     0.0737421926
  C4       -0.6642570925     3.2520488836    -0.6367052685
  C5       -0.4176006880     3.7506626636     0.6266617261
  C6        0.3544512795     1.5880350880     1.3466103113
  C7        0.4170777837    -0.3985715830    -0.1699592855
  H3       -1.0525605122     3.8885742810    -1.4118210930
  H4       -0.6167322086     4.7833170549     0.8545293591
  H6        0.2674814541     3.3270622399     2.5955278254
  H7        1.4973945803    -0.4731027075    -0.3024150114
  C10      -0.2287965646    -0.9806639283    -1.4178880613
  C8        0.0698890241    -1.2028043787     1.1012482231
```

```
  C16       0.3878450683     -2.6927505821      0.9926362549
  H12      -0.9951779944     -1.0820840286      1.2983596370
  N2        0.9170358115      0.7553208143      2.3370671452
  C9        0.7768072859     -0.6080366017      2.3120223174
  C17       1.5610950577      1.3485102001      3.5009099154
  O1        1.1832216246     -1.2932589235      3.2054919248
  C11      -1.3897408665     -2.0946804498     -3.7076261186
  C12       0.5573168988     -1.4058899863     -2.4785095426
  C13      -1.6134753191     -1.1154172400     -1.5247167612
  C14      -2.1880030799     -1.6684722289     -2.6547607738
  C15      -0.0160431399     -1.9591481309     -3.6166482122
  H19       1.6281608801     -1.3085902778     -2.4194149758
  H20      -2.2471717937     -0.7784529708     -0.7228773625
  H21      -3.2581532808     -1.7658803019     -2.7164491956
  H22       0.6138580213     -2.2836317578     -4.4266535536
  H23      -1.8366797945     -2.5253223675     -4.5869058888
  H24       1.4388793077     -2.8469283504      0.7688543441
  H25      -0.1976502735     -3.1491850817      0.2053308323
  H11       0.1740858417     -3.1922226846      1.9269623073
  H2        2.1959879407      2.1661330306      3.1833633143
  H5        2.1568809098      0.5930508704      3.9824096527
  H8        0.8333257979      1.7217187718      4.2134231671

  nuclear repulsion energy.......  1393.834798082 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   9   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.318E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
82
  grid # 2      113     96     96     98     97     97     93
91
  grid # 3      213    184    183    192    183    183    193
175
```

```
  grid # 4      213    327    328    338    327    328    327
311

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     67     90     82     74
68
  grid # 2      118    118    112    105    100     91     80
111
  grid # 3      223    223    207    209    192    176    147
213
  grid # 4      224    223    208    206    339    309    287
208

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       94     81     72    111     89     87     87
89
  grid # 2      104     92     79    123     97     95     95
95
  grid # 3      213    176    142    257    182    182    183
183
  grid # 4      390    291    272    450    326    326    326
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     70     73     73     73     71
71
  grid # 2       97    113    113    118    118    118    109
110
  grid # 3      182    213    212    223    223    224    218
215
  grid # 4      326    213    210    223    224    224    219
213

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       70     71     70     71   2862
  grid # 2      108    111    107    111   3729
  grid # 3      218    215    213    217   7187
  grid # 4      214    212    209    217   9914

  end of program grid


  start of program rwr
  end of program rwr
```

```
  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS     maximum
      e  d  i  u  i                        energy   density    DIIS
      r  t  s  t  d     total energy       change   change     error

etot  1  N  N  1  U  -783.03124326647                 2.4E-04  3.6E-03
etot  2  Y  Y  4  M  -783.03397401455  2.7E-03        6.0E-05  1.4E-03
etot  3  Y  Y  4  M  -783.03429532404  3.2E-04        1.3E-05  3.4E-04
etot  4  N  Y  1  U  -783.03431616083  2.1E-05        9.6E-06  1.7E-04
etot  5  Y  Y  4  M  -783.03432088914  4.7E-06        3.9E-06  6.6E-05
etot  6  Y  N  4  M  -783.03432006507 -8.2E-07        0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1393.83479808193
   (E)  Total one-electron terms..... -3832.15009804478
   (I)  Total two-electron terms.....  1655.28097989779
   (L)  Electronic energy............. -2176.86911814699  (E+I)
   (N)  Total energy.................  -783.03432006507  (A+L)

 SCFE: SCF energy: HF    -783.03432006507 hartrees   iterations:
6


 HOMO energy:    -0.30084
 LUMO energy:     0.12741

  Orbital energies:
  -20.52620  -15.59981  -11.34556  -11.28396  -11.25517  -11.25116
  -11.24395  -11.24304  -11.24149  -11.23660  -11.23646  -11.23611
  -11.23404  -11.23384  -11.23383  -11.23354  -11.23238  -11.22719
  -11.20740   -1.39895   -1.26899   -1.16894   -1.14816   -1.10688
   -1.03058   -1.02018   -1.01838   -1.01508   -0.95990   -0.93288
   -0.85912   -0.83796   -0.83170   -0.82989   -0.78964   -0.74345
   -0.71209   -0.69629   -0.68088   -0.66514   -0.64197   -0.63615
   -0.62751   -0.61860   -0.61259   -0.60451   -0.59818   -0.58820
   -0.57058   -0.56067   -0.54980   -0.54047   -0.52885   -0.52100
   -0.51450   -0.50485   -0.49988   -0.49678   -0.48375   -0.47054
   -0.46822   -0.42024   -0.41266   -0.34284   -0.33565   -0.32745
   -0.30084    0.12741    0.13710    0.14173    0.15153    0.20432
    0.23548    0.24203    0.25336    0.26137    0.27468

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	1.860102E-04	2.065891E-04	6.481016E-04
2	C1	-1.195764E-04	-2.838357E-04	-6.501493E-04
3	C2	5.172992E-05	8.031919E-04	6.697169E-04
4	C3	-1.711775E-04	2.453431E-05	-9.632215E-05
5	C4	-2.263973E-04	6.377435E-04	-6.824798E-05
6	C5	-1.901842E-04	2.904630E-04	-3.555040E-04
7	C6	2.682721E-04	-3.775273E-04	-1.403175E-04
8	C7	5.315907E-04	-2.037355E-04	1.311403E-04
9	H3	9.301685E-05	-6.531298E-05	1.743987E-04
10	H4	-4.474642E-05	-1.723562E-04	-1.568821E-04
11	H6	-1.754128E-04	-3.073676E-04	-5.985968E-04
12	H7	-5.866506E-04	3.421160E-05	-3.750699E-05
13	C10	-8.190485E-04	8.372074E-05	1.125955E-04
14	C8	-2.573597E-04	3.550686E-04	2.625775E-05
15	C16	1.888017E-04	-3.063027E-04	9.169531E-05
16	H12	-9.271932E-05	6.021564E-05	-5.580567E-05
17	N2	-3.872001E-06	-3.801622E-05	3.467940E-04
18	C9	-8.431177E-04	2.330484E-03	-3.153583E-03
19	C17	4.859849E-04	5.341231E-04	-7.721778E-04
20	O1	1.160628E-03	-2.878854E-03	3.348444E-03
21	C11	8.396801E-04	-1.059340E-04	-3.874763E-04
22	C12	5.545321E-05	-2.641235E-04	-5.216739E-04
23	C13	3.778033E-04	6.269344E-05	5.148744E-05
24	C14	-1.493969E-04	2.565743E-04	4.807514E-04
25	C15	-3.390704E-04	-4.628016E-05	-2.185419E-04
26	H19	-2.508413E-04	-6.985398E-05	2.026653E-06
27	H20	3.829492E-05	-3.969604E-05	-2.971585E-05
28	H21	1.966670E-04	8.326767E-05	1.013774E-04
29	H22	-5.999626E-05	3.946104E-05	1.112738E-04
30	H23	1.940068E-04	1.475429E-04	2.894697E-04
31	H24	1.335069E-04	3.551797E-05	-1.687080E-05
32	H25	-1.931937E-04	-1.115342E-04	-7.408061E-05
33	H11	-6.403831E-05	7.979125E-05	-2.925790E-05
34	H2	-8.910387E-05	-1.994286E-04	9.318523E-05
35	H5	6.360593E-05	-1.926116E-04	-1.323588E-04
36	H8	-5.292874E-04	1.604759E-04	4.777059E-04
total		-3.401377E-04	5.629000E-04	-3.386478E-04

```
 end of program der1b
```

```
  start of program geopt  10

  geometry optimization step 10
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:           1.8305E-06 #  (  5.0000E-05 )
  gradient maximum:        4.5629E-03 .  (  4.5000E-04 )
  gradient rms:            5.0397E-04 .  (  3.0000E-04 )
  step size:   0.03869  trust radius:   0.30000
  displacement maximum:    1.7978E-02 .  (  1.8000E-03 )
  displacement rms:        3.5033E-03 .  (  1.2000E-03 )
  predicted energy change:    -2.7620E-05    geom step:   3.8695E-
02    full step:   3.8695E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.3728E-03     y:     6.4620E-05     z:     8.4566E-04

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -0.6078392891     1.5257285909    -1.8816305007
  C1       -0.4147302906     1.9137246270    -0.8996660553
  C2        0.0857348227     2.9227360072     1.6185727975
  C3        0.0923789062     1.0683075800     0.0727830963
  C4       -0.6738447489     3.2507314171    -0.6334863392
  C5       -0.4268019504     3.7487534664     0.6300124967
  C6        0.3576187179     1.5883593416     1.3451887258
  C7        0.4163634610    -0.3994704181    -0.1681753778
  H3       -1.0662753637     3.8867215880    -1.4064765862
  H4       -0.6314135796     4.7797403324     0.8591356889
  H6        0.2644285629     3.3240296078     2.5968451898
  H7        1.4960420487    -0.4755128303    -0.2968573232
  C10      -0.2260049617    -0.9817660355    -1.4178557163
  C8        0.0633005965    -1.2001103120     1.1039223674
  C16       0.3744436051    -2.6925058953     0.9987930688
  H12      -1.0015430019    -1.0739635866     1.2991883729
  N2        0.9258266093     0.7550127080     2.3321143356
  C9        0.7714055444    -0.6067833391     2.3145562494
  C17       1.5822316824     1.3482739795     3.4886284863
  O1        1.1640414096    -1.2941795255     3.2155442382
  C11      -1.3787368361    -2.0920353232    -3.7124020855
  C12       0.5634583814    -1.4066069283    -2.4771894323
  C13      -1.6097696264    -1.1162196731    -1.5280304928
  C14      -2.1803878157    -1.6672081682    -2.6604467317
  C15      -0.0058123642    -1.9576859369    -3.6179949724
  H19       1.6338991581    -1.3102539622    -2.4143742672
  H20      -2.2457892220    -0.7809943209    -0.7274668312
```

```
  H21      -3.2501428427     -1.7642912954     -2.7249712957
  H22       0.6264860420     -2.2811666380     -4.4262332624
  H23      -1.8234640970     -2.5208057986     -4.5929780329
  H24       1.4240326077     -2.8522883044      0.7711151093
  H25      -0.2168556307     -3.1491798774      0.2156647316
  H11       0.1615794593     -3.1873685160      1.9356277210
  H2        2.2066290864      2.1704345145      3.1641607099
  H5        2.1902735396      0.5938499752      3.9577522952
  H8        0.8621805535      1.7135991017      4.2152328195

  nuclear repulsion energy.......  1393.740001573 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  10   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.325E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
82
  grid # 2      113     96     96     98     97     97     93
91
  grid # 3      213    184    183    192    183    183    191
175
  grid # 4      212    327    328    339    327    328    327
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     67     92     83     74
68
  grid # 2      118    118    112    106    100     91     80
110
  grid # 3      223    223    207    209    192    176    145
212
```

```
  grid # 4      224    223    208    205    337    309    287
208

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       94     81     70    111     89     87     87
89
  grid # 2      104     93     79    123     97     95     95
95
  grid # 3      213    176    143    257    182    182    183
183
  grid # 4      389    292    272    450    326    326    326
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     70     73     73     73     71
71
  grid # 2       97    113    113    118    118    118    110
110
  grid # 3      182    213    212    223    223    224    218
214
  grid # 4      326    213    210    223    224    224    219
213

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       71     71     70     71   2864
  grid # 2      108    111    108    111   3732
  grid # 3      218    215    213    217   7182
  grid # 4      214    213    209    218   9914

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                          RMS    maximum
      t  p  i  c  r                                 energy density   DIIS
      e  d  i  u  i                  total energy   change change    error

etot  1  N  N  1  U  -783.03394136022                      4.9E-05  1.2E-03
etot  2  Y  Y  4  M  -783.03429225493  3.5E-04  2.0E-05  4.9E-04
etot  3  Y  Y  4  M  -783.03433295116  4.1E-05  4.7E-06  1.2E-04
etot  4  Y  N  4  M  -783.03433544023  2.5E-06  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1393.74000157308
   (E)  Total one-electron terms..... -3831.96028880495
   (I)  Total two-electron terms.....  1655.18595179163
   (L)  Electronic energy..... -2176.77433701331  (E+I)
   (N)  Total energy.............  -783.03433544023  (A+L)

 SCFE: SCF energy: HF    -783.03433544023 hartrees   iterations:
4


 HOMO energy:    -0.30113
 LUMO energy:     0.12745

  Orbital energies:
 -20.52664  -15.59996  -11.34573  -11.28413  -11.25558  -11.25097
 -11.24382  -11.24304  -11.24173  -11.23663  -11.23657  -11.23601
 -11.23401  -11.23383  -11.23369  -11.23347  -11.23264  -11.22730
 -11.20752   -1.39750   -1.26910   -1.16892   -1.14816   -1.10677
  -1.03045   -1.02004   -1.01865   -1.01520   -0.95992   -0.93285
  -0.85916   -0.83805   -0.83181   -0.82993   -0.78971   -0.74360
  -0.71203   -0.69625   -0.68093   -0.66510   -0.64201   -0.63608
  -0.62743   -0.61881   -0.61235   -0.60464   -0.59799   -0.58834
  -0.57059   -0.56056   -0.55009   -0.54029   -0.52856   -0.52089
  -0.51452   -0.50478   -0.49997   -0.49672   -0.48367   -0.47053
  -0.46818   -0.42005   -0.41270   -0.34297   -0.33542   -0.32757
  -0.30113    0.12745    0.13707    0.14161    0.15147    0.20359
   0.23548    0.24206    0.25342    0.26127    0.27477

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1     -7.810709E-05  -8.964953E-05  -1.985821E-04
   2    C1      3.812288E-05   3.842454E-05   1.624278E-04
   3    C2     -1.219649E-04   6.408960E-05  -3.043236E-04
   4    C3      8.842063E-05   1.756709E-05   3.326705E-04
```

5	C4	2.756740E-05	1.663489E-04	1.991776E-04
6	C5	5.528171E-05	-1.760322E-04	-1.639682E-04
7	C6	-1.936015E-04	-6.266329E-05	-7.170922E-04
8	C7	-1.126598E-04	1.266528E-04	-1.520178E-05
9	H3	1.270036E-05	4.947748E-05	-6.250118E-05
10	H4	1.377330E-05	5.069176E-05	-1.920233E-05
11	H6	4.409932E-05	8.452816E-05	1.142472E-04
12	H7	4.614525E-05	3.815257E-06	-4.714894E-05
13	C10	1.387159E-04	-6.290560E-05	-1.149535E-04
14	C8	-1.032740E-04	-7.459522E-05	-2.573135E-04
15	C16	9.782985E-06	-5.294055E-05	-3.057395E-05
16	H12	-2.224320E-05	1.707269E-05	-2.357005E-05
17	N2	7.689911E-05	-1.504170E-04	5.062423E-04
18	C9	-5.122361E-04	-1.334435E-05	-1.831681E-04
19	C17	-1.547649E-04	-1.239781E-04	3.338134E-04
20	O1	5.592852E-04	3.074811E-04	2.436664E-04
21	C11	-1.585779E-04	1.220829E-04	2.861336E-04
22	C12	-8.877638E-05	1.520934E-04	2.839581E-04
23	C13	2.040256E-04	3.845181E-05	-3.802457E-05
24	C14	1.093739E-04	-1.629729E-04	-4.053137E-04
25	C15	-2.547229E-04	3.516358E-05	8.338680E-05
26	H19	-3.314051E-05	2.615021E-05	5.911915E-05
27	H20	3.148182E-06	2.537441E-05	3.128719E-05
28	H21	3.609963E-05	2.844231E-06	-2.611290E-05
29	H22	2.184836E-06	-1.277204E-05	-1.439460E-05
30	H23	-3.497067E-05	-2.946945E-05	-5.724033E-05
31	H24	-3.684495E-05	6.332792E-05	2.707429E-05
32	H25	-1.823871E-05	1.198512E-05	-6.748054E-05
33	H11	-9.700306E-06	6.765797E-05	-1.014622E-08
34	H2	8.353946E-05	6.815708E-05	7.393435E-05
35	H5	-1.453759E-04	1.442796E-04	-6.724910E-05
36	H8	2.091747E-04	-1.272725E-04	-2.382149E-04
total		-3.208593E-04	5.447050E-04	-3.145015E-04

end of program der1b

start of program geopt 11

geometry optimization step 11
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format

energy change: -1.5375E-05 * (5.0000E-05)
gradient maximum: 1.2333E-03 . (4.5000E-04)
gradient rms: 2.0840E-04 * (3.0000E-04)

```
  step size:   0.03638  trust radius:   0.30000
  displacement maximum:    2.0266E-02 .  (  1.8000E-03 )
  displacement rms:        3.2941E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.1420E-05    geom step:   3.6384E-
02    full step:   3.6384E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.6121E-03     y:    -8.7558E-05     z:    -6.0102E-04

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -0.5935984515      1.5253691277     -1.8860561063
  C1       -0.4050751086      1.9139654377     -0.9031715306
  C2        0.0823834468      2.9228330418      1.6168993776
  C3        0.0954787344      1.0677644296      0.0724622424
  C4       -0.6633365950      3.2516270972     -0.6395503974
  C5       -0.4226094703      3.7494219990      0.6252116845
  C6        0.3540879810      1.5874470606      1.3460276235
  C7        0.4198918222     -0.3994939817     -0.1702937839
  H3       -1.0497886920      3.8879451275     -1.4152883120
  H4       -0.6262193555      4.7809687202      0.8528463009
  H6        0.2563777084      3.3245195032      2.5959630361
  H7        1.4989383697     -0.4746539180     -0.3040493579
  C10      -0.2276497686     -0.9810661092     -1.4175937392
  C8        0.0718055401     -1.2031033148      1.1009170664
  C16       0.3897297154     -2.6940199746      0.9924578794
  H12      -0.9936546052     -1.0821648706      1.2971479889
  N2        0.9159418981      0.7549076380      2.3382065804
  C9        0.7777827727     -0.6082483248      2.3123104480
  C17       1.5610183486      1.3495244786      3.5002472528
  O1        1.1818495681     -1.2955168580      3.2085577821
  C11      -1.3913991842     -2.0907496943     -3.7064117421
  C12       0.5570206560     -1.4096326614     -2.4786017058
  C13      -1.6120364124     -1.1114101672     -1.5230623473
  C14      -2.1881783311     -1.6620695393     -2.6527680554
  C15      -0.0178454719     -1.9605007339     -3.6165968112
  H19       1.6279564470     -1.3165981585     -2.4190088528
  H20      -2.2442506448     -0.7730900942     -0.7207351840
  H21      -3.2584089317     -1.7558839400     -2.7135462368
  H22       0.6108601570     -2.2872224102     -4.4263852447
  H23      -1.8402333775     -2.5195647362     -4.5849195054
  H24       1.4407638362     -2.8481397350      0.7668669450
  H25      -0.1980556518     -3.1514150949      0.2065910963
  H11       0.1768254931     -3.1919938480      1.9277513551
  H2        2.1900224789      2.1711694553      3.1829814548
  H5        2.1629334047      0.5947946533      3.9764857450
  H8        0.8329033950      1.7155544758      4.2181598779

  nuclear repulsion energy.......  1393.761377017 hartrees
  ------------------------------------------------
```

```
 /  end of geometry optimization iteration  11   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.324E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
82
  grid # 2      113     96     96     98     97     97     93
91
  grid # 3      213    184    184    192    183    183    195
175
  grid # 4      213    327    328    338    327    328    328
311

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     66     91     83     73
68
  grid # 2      118    118    112    106    100     91     80
111
  grid # 3      223    223    207    209    192    176    146
212
  grid # 4      224    223    208    206    337    309    286
208

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       94     81     70    111     89     87     87
89
  grid # 2      103     93     79    123     97     95     95
95
  grid # 3      212    176    141    257    182    182    183
183
```

```
  grid # 4      389    293    272    450    326    326    326
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     70     73     73     73     71
71
  grid # 2       97    113    113    118    118    118    110
110
  grid # 3      182    213    212    223    223    224    218
214
  grid # 4      326    213    210    223    224    224    219
213

  number of gridpoints:
     atom       H11     H2     H5     H8  total
  grid # 1       71     71     70     71   2861
  grid # 2      108    111    108    111   3732
  grid # 3      218    215    213    217   7185
  grid # 4      214    213    209    218   9915

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03399209554           4.6E-05  9.9E-04
etot   2  Y  Y  4  M  -783.03430321865  3.1E-04  1.8E-05  4.1E-04
etot   3  Y  Y  4  M  -783.03433735612  3.4E-05  4.6E-06  1.2E-04
etot   4  Y  N  4  M  -783.03434086354  3.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1393.76137701651
   (E)  Total one-electron terms..... -3831.99987497203
   (I)  Total two-electron terms.....  1655.20415709198
   (L)  Electronic energy............. -2176.79571788005  (E+I)
   (N)  Total energy.................  -783.03434086354  (A+L)

 SCFE: SCF energy: HF    -783.03434086354 hartrees   iterations:
4
```

```
HOMO energy:    -0.30113
LUMO energy:     0.12734

 Orbital energies:
 -20.52561  -15.60069  -11.34598  -11.28452  -11.25546  -11.25116
 -11.24377  -11.24335  -11.24177  -11.23650  -11.23649  -11.23602
 -11.23396  -11.23386  -11.23367  -11.23340  -11.23267  -11.22725
 -11.20762   -1.39725   -1.26906   -1.16909   -1.14822   -1.10690
  -1.03050   -1.02015   -1.01867   -1.01518   -0.96004   -0.93288
  -0.85917   -0.83814   -0.83184   -0.82997   -0.78982   -0.74353
  -0.71215   -0.69629   -0.68095   -0.66501   -0.64197   -0.63621
  -0.62759   -0.61863   -0.61220   -0.60455   -0.59837   -0.58837
  -0.57053   -0.56074   -0.54985   -0.54025   -0.52856   -0.52088
  -0.51453   -0.50487   -0.49997   -0.49676   -0.48374   -0.47053
  -0.46822   -0.42011   -0.41260   -0.34303   -0.33555   -0.32746
  -0.30113    0.12734    0.13695    0.14163    0.15143    0.20381
   0.23554    0.24202    0.25330    0.26130    0.27467

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H1     -5.038272E-05  -3.430879E-06  -4.127185E-05
  2    C1      4.748965E-05   1.436707E-05   8.927109E-05
  3    C2      3.883389E-05  -1.767239E-04  -1.390654E-04
  4    C3     -1.960406E-05   9.362188E-05   3.028842E-05
  5    C4      4.797557E-05  -9.604501E-05   1.187475E-04
  6    C5      9.352827E-06  -2.287114E-05  -7.718446E-05
  7    C6     -8.233836E-05   9.440645E-05   6.572687E-06
  8    C7     -1.291833E-04   3.833985E-05  -6.946861E-05
  9    H3     -6.231702E-05   5.146157E-05  -3.933181E-05
 10    H4     -3.415629E-05   4.792490E-05  -7.092552E-07
 11    H6      2.078378E-05   6.600199E-05   1.001699E-05
 12    H7      1.004260E-04  -3.494904E-06   1.723556E-05
 13    C10     6.574826E-05   1.081940E-05  -8.635306E-07
 14    C8     -7.916145E-05  -6.733571E-05   7.370609E-05
 15    C16    -4.835523E-05   2.554411E-05  -7.266745E-05
 16    H12     1.132747E-04   9.984863E-06  -5.333502E-05
```

17	N2	2.611538E-05	1.790270E-04	-4.273302E-04
18	C9	-2.244819E-04	8.988192E-05	-1.428135E-04
19	C17	-2.270077E-05	-1.772595E-04	3.678360E-04
20	O1	3.138213E-05	-3.691366E-05	1.640488E-04
21	C11	-3.910250E-05	6.374560E-06	2.450221E-06
22	C12	3.346522E-05	1.069812E-04	1.836707E-04
23	C13	6.953073E-05	6.251142E-05	8.647149E-05
24	C14	-5.576443E-05	-8.132873E-05	-1.537285E-04
25	C15	-7.550831E-05	-2.866128E-05	-7.673363E-05
26	H19	-3.401630E-05	1.645046E-05	6.883913E-06
27	H20	3.427838E-06	1.245798E-05	-9.792845E-06
28	H21	-1.879148E-05	-3.616275E-06	-3.593808E-05
29	H22	-2.482896E-05	2.591086E-06	-1.608591E-05
30	H23	-2.822671E-05	-9.722769E-06	-7.631009E-05
31	H24	-1.578005E-04	1.157382E-05	5.086852E-05
32	H25	1.030225E-04	1.167702E-04	1.408885E-04
33	H11	4.589712E-05	1.998409E-05	-3.581901E-05
34	H2	-1.374699E-05	2.739294E-05	-3.050550E-05
35	H5	-4.836191E-05	1.793460E-04	-5.284020E-05
36	H8	1.808844E-04	-1.504161E-05	-1.184863E-04
total		-3.112191E-04	5.613693E-04	-3.213246E-04

end of program der1b

start of program geopt 12

geometry optimization step 12
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format

energy change: -5.4233E-06 * (5.0000E-05)
gradient maximum: 4.7893E-04 . (4.5000E-04)
gradient rms: 1.0732E-04 * (3.0000E-04)
step size: 0.02080 trust radius: 0.30000
displacement maximum: 9.7038E-03 . (1.8000E-03)
displacement rms: 1.8830E-03 . (1.2000E-03)
predicted energy change: -5.7667E-06 geom step: 2.0799E-02 full step: 2.0799E-02
molecular structure not yet converged...

center of mass moved by:
x: -8.0623E-04 y: 1.4286E-04 z: 1.2430E-04

new geometry:
angstroms

```
 atom            x                 y                 z
 H1       -0.6073568924      1.5237136662     -1.8823399573
 C1       -0.4132574313      1.9129243655     -0.9005300812
 C2        0.0878291597      2.9236936494      1.6160967077
 C3        0.0920755393      1.0676189110      0.0732141482
 C4       -0.6695794665      3.2508310669     -0.6365785660
 C5       -0.4216073809      3.7497692671      0.6262090355
 C6        0.3564609800      1.5881448103      1.3450742509
 C7        0.4161138831     -0.3998697248     -0.1682736666
 H3       -1.0603332588      3.8865832498     -1.4107872708
 H4       -0.6232329737      4.7816742453      0.8540560776
 H6        0.2674993205      3.3262548416      2.5940031000
 H7        1.4956872174     -0.4753405691     -0.2990005913
 C10      -0.2276672535     -0.9820444319     -1.4171249084
 C8        0.0657510594     -1.2018427690      1.1034857617
 C16       0.3804762605     -2.6934469230      0.9970964098
 H12      -0.9991567848     -1.0781218244      1.2996674453
 N2        0.9212477978      0.7551906248      2.3349277741
 C9        0.7740209648     -0.6071958928      2.3137354032
 C17       1.5719093168      1.3480710312      3.4950812853
 O1        1.1748254874     -1.2936705069      3.2119780506
 C11      -1.3837488082     -2.0909193702     -3.7107852685
 C12       0.5602748554     -1.4052326613     -2.4777006917
 C13      -1.6115270524     -1.1174213169     -1.5254865725
 C14      -2.1838631314     -1.6677719413     -2.6575562630
 C15      -0.0106969357     -1.9556214346     -3.6180434299
 H19       1.6307522154     -1.3081187291     -2.4162425044
 H20      -2.2464479112     -0.7832653688     -0.7235119593
 H21      -3.2536501932     -1.7654498939     -2.7204868024
 H22       0.6206515471     -2.2779785309     -4.4276036183
 H23      -1.8293204095     -2.5192695432     -4.5913177455
 H24       1.4309150715     -2.8501048232      0.7716830167
 H25      -0.2080273356     -3.1504446869      0.2120838127
 H11       0.1670804496     -3.1896659673      1.9330464800
 H2        2.1996274802      2.1697910415      3.1750570863
 H5        2.1760208716      0.5931629668      3.9679968304
 H8        0.8478444334      1.7139257544      4.2165621306

 nuclear repulsion energy.......  1393.740051355 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  12   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.322E-04
 number of canonical orbitals.....          368
 end of program onee
```

```
  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
82
  grid # 2      113     96     96     98     97     97     93
91
  grid # 3      213    184    183    192    183    183    195
175
  grid # 4      212    327    328    338    327    328    328
311

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C16
H12
  grid # 1       73     73     70     67     90     82     74
68
  grid # 2      118    118    112    106    100     91     80
111
  grid # 3      223    223    207    209    192    176    145
212
  grid # 4      224    223    208    205    337    309    287
208

  number of gridpoints:
     atom        N2     C9    C17     O1    C11    C12    C13
C14
  grid # 1       94     81     70    111     89     87     87
89
  grid # 2      103     93     79    123     97     95     95
95
  grid # 3      213    176    142    257    182    182    183
183
  grid # 4      389    291    272    450    326    326    326
326

  number of gridpoints:
     atom       C15    H19    H20    H21    H22    H23    H24
H25
  grid # 1       89     73     70     73     73     73     71
71
  grid # 2       97    113    113    118    118    118    110
110
  grid # 3      182    213    212    223    223    224    218
214
```

```
  grid # 4      326    213    210    223    224    224    219
213

  number of gridpoints:
     atom       H11     H2      H5      H8  total
  grid # 1       71     71      70      71   2861
  grid # 2      108    111     107     111   3731
  grid # 3      218    215     213     217   7185
  grid # 4      214    213     209     218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                          energy  density   DIIS
       e  d  i  u  i                          change  change    error
       r  t  s  t  d     total energy

etot   1  N  N  1  U  -783.03420083779           3.0E-05  6.8E-04
etot   2  Y  Y  4  M  -783.03432692125  1.3E-04  1.2E-05  2.3E-04
etot   3  Y  Y  4  M  -783.03434327005  1.6E-05  3.3E-06  7.6E-05
etot   4  Y  N  4  M  -783.03434219864 -1.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1393.74005135506
   (E)  Total one-electron terms..... -3831.96157079990
   (I)  Total two-electron terms.....  1655.18717724620
   (L)  Electronic energy............. -2176.77439355370  (E+I)
   (N)  Total energy.................  -783.03434219864  (A+L)

 SCFE: SCF energy: HF    -783.03434219864 hartrees   iterations:
4


 HOMO energy:    -0.30110
 LUMO energy:     0.12736

  Orbital energies:
  -20.52629  -15.59998  -11.34569  -11.28403  -11.25537  -11.25102
  -11.24382  -11.24313  -11.24165  -11.23661  -11.23657  -11.23608
  -11.23396  -11.23396  -11.23378  -11.23350  -11.23257  -11.22737
  -11.20752   -1.39737   -1.26883   -1.16902   -1.14822   -1.10684
   -1.03051   -1.02016   -1.01862   -1.01517   -0.95989   -0.93289
   -0.85914   -0.83801   -0.83184   -0.82996   -0.78973   -0.74350
   -0.71209   -0.69627   -0.68087   -0.66504   -0.64195   -0.63613
```

```
 -0.62750   -0.61870   -0.61228   -0.60455   -0.59811   -0.58833
 -0.57059   -0.56064   -0.54988   -0.54027   -0.52854   -0.52088
 -0.51455   -0.50485   -0.50000   -0.49677   -0.48370   -0.47052
 -0.46820   -0.42005   -0.41264   -0.34295   -0.33552   -0.32757
 -0.30110    0.12736    0.13705    0.14164    0.15147    0.20379
  0.23548    0.24206    0.25337    0.26129    0.27469

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	8.071198E-05	5.095699E-05	1.424365E-04
2	C1	-2.842678E-06	-4.917564E-05	-1.711653E-04
3	C2	-6.775573E-05	2.291933E-04	6.024684E-05
4	C3	-4.577852E-05	-5.221800E-05	-1.224681E-04
5	C4	-1.921893E-05	5.813724E-05	1.504679E-06
6	C5	-1.101094E-05	1.617310E-05	-4.292541E-05
7	C6	4.463637E-05	-1.819969E-05	4.260803E-05
8	C7	-1.199106E-05	-1.777390E-05	-3.028820E-05
9	H3	5.587173E-05	-1.136255E-05	3.755564E-05
10	H4	-2.495721E-05	1.658040E-06	-2.760971E-05
11	H6	-7.568571E-05	-1.969821E-05	-9.262860E-05
12	H7	-8.305769E-06	2.404577E-05	-9.072828E-06
13	C10	-1.985094E-04	3.753055E-05	2.541633E-05
14	C8	3.736078E-05	3.021919E-06	-2.427377E-06
15	C16	2.267186E-05	1.041961E-04	2.185742E-05
16	H12	-4.842537E-05	2.536326E-05	-3.649629E-06
17	N2	-4.511609E-05	4.321185E-05	4.582465E-05
18	C9	4.064552E-06	5.584315E-06	-1.285220E-04
19	C17	1.141878E-04	1.034934E-04	-5.695981E-05
20	O1	2.257018E-05	-1.393803E-04	1.041672E-04
21	C11	1.550269E-04	-1.835205E-06	-3.722847E-05
22	C12	4.945254E-06	-7.152869E-06	-1.716240E-05
23	C13	9.103410E-05	5.839915E-05	1.876719E-05
24	C14	1.790959E-05	2.983951E-05	7.641090E-07
25	C15	-1.323647E-04	-4.695856E-05	-6.696346E-05
26	H19	-4.809622E-05	-2.206898E-05	5.851227E-06
27	H20	1.625447E-05	2.343135E-05	-3.091705E-05
28	H21	1.862995E-05	3.121685E-05	-1.051434E-05

```
 29    H22    -4.533792E-05  -1.040017E-05   4.262036E-05
 30    H23     1.168462E-05   1.928602E-05   2.738866E-05
 31    H24     9.246487E-06   2.178443E-05  -3.255970E-06
 32    H25    -4.989110E-05  -1.260823E-05  -2.334741E-05
 33    H11    -2.932134E-05   1.038159E-07   2.449929E-05
 34    H2     -5.901152E-05  -5.502665E-05   2.687955E-05
 35    H5     -7.597745E-05   7.866496E-05  -9.679017E-05
 36    H8     -4.316473E-05   3.822545E-05   2.457594E-05
-----------   -------------  -------------  -------------
   total      -3.359558E-04   5.396585E-04  -3.209327E-04

 end of program der1b


 start of program geopt  13

 geometry optimization step 13
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:          -1.3351E-06 #  (  5.0000E-05 )
 gradient maximum:        2.7004E-04 *  (  4.5000E-04 )
 gradient rms:            7.9770E-05 *  (  3.0000E-04 )
 step size:   0.01152  trust radius:   0.30000
 displacement maximum:    6.1467E-03 .  (  1.8000E-03 )
 displacement rms:        1.0432E-03 *  (  1.2000E-03 )
 predicted energy change:    -2.7211E-06    geom step:   1.1522E-
02    full step:   1.1522E-02

 ***************************************************
 **           Geometry optimization complete          **
 ***************************************************

 center of mass moved by:
    x:     0.0000E+00     y:     0.0000E+00     z:     0.0000E+00

 final geometry:
                                angstroms
 atom            x                 y                 z
 H1       -0.6073568924      1.5237136662     -1.8823399573
 C1       -0.4132574313      1.9129243655     -0.9005300812
 C2        0.0878291597      2.9236936494      1.6160967077
 C3        0.0920755393      1.0676189110      0.0732141482
 C4       -0.6695794665      3.2508310669     -0.6365785660
 C5       -0.4216073809      3.7497692671      0.6262090355
 C6        0.3564609800      1.5881448103      1.3450742509
 C7        0.4161138831     -0.3998697248     -0.1682736666
```

```
 H3       -1.0603332588      3.8865832498     -1.4107872708
 H4       -0.6232329737      4.7816742453      0.8540560776
 H6        0.2674993205      3.3262548416      2.5940031000
 H7        1.4956872174     -0.4753405691     -0.2990005913
 C10      -0.2276672535     -0.9820444319     -1.4171249084
 C8        0.0657510594     -1.2018427690      1.1034857617
 C16       0.3804762605     -2.6934469230      0.9970964098
 H12      -0.9991567848     -1.0781218244      1.2996674453
 N2        0.9212477978      0.7551906248      2.3349277741
 C9        0.7740209648     -0.6071958928      2.3137354032
 C17       1.5719093168      1.3480710312      3.4950812853
 O1        1.1748254874     -1.2936705069      3.2119780506
 C11      -1.3837488082     -2.0909193702     -3.7107852685
 C12       0.5602748554     -1.4052326613     -2.4777006917
 C13      -1.6115270524     -1.1174213169     -1.5254865725
 C14      -2.1838631314     -1.6677719413     -2.6575562630
 C15      -0.0106969357     -1.9556214346     -3.6180434299
 H19       1.6307522154     -1.3081187291     -2.4162425044
 H20      -2.2464479112     -0.7832653688     -0.7235119593
 H21      -3.2536501932     -1.7654498939     -2.7204868024
 H22       0.6206515471     -2.2779785309     -4.4276036183
 H23      -1.8293204095     -2.5192695432     -4.5913177455
 H24       1.4309150715     -2.8501048232      0.7716830167
 H25      -0.2080273356     -3.1504446869      0.2120838127
 H11       0.1670804496     -3.1896659673      1.9330464800
 H2        2.1996274802      2.1697910415      3.1750570863
 H5        2.1760208716      0.5931629668      3.9679968304
 H8        0.8478444334      1.7139257544      4.2165621306

 nuclear repulsion energy.......  1393.740051355 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  13   /
-------------------------------------------------

 end of program geopt


 start of program post
 Writing a SPARTAN archive file
 end of program post

Total cpu seconds     user:     962.281   user+sys:     962.281
```

CIS 1 (PH_AX – ME_EQ)

```
+-----------------------------------------------------------------
---+
  |  Jaguar version 3.5, release  42
|
  |
|
  |  Copyright 1991-1998 Schrodinger, Inc.
|
  |  All Rights Reserved.
|
  |
|
  |  Use of this program should be acknowledged in publications
as:    |
  |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.
|
  +-----------------------------------------------------------------
-----+

  start of program pre
  Job name: WF32484
  Executables used: D:\TITAN
  Temporary files : C:\Users\gfabr\AppData\Local\Temp\WF32484

  Input file comments:
    Molecule001
    This file created by Spartan

  basis set:             6-31G**
  net molecular charge:    0
  multiplicity:            1

  number of basis functions....          370

 Input geometry:
                                 angstroms
  atom            x                  y                  z
  H1       -1.0908480000      1.8329980000     -2.2644300000
  C1       -1.0340050000      2.0777930000     -1.1971850000
  C2       -0.8848920000      2.7070200000      1.5066230000
  C3       -0.8895200000      1.0499730000     -0.2640980000
  C4       -1.1023190000      3.4031230000     -0.7887820000
  C5       -1.0277110000      3.7150800000      0.5649260000
  C6       -0.8128850000      1.3653830000      1.1030560000
  C7       -0.8287630000     -0.3712940000     -0.7489220000
  H3       -1.2147720000      4.1999660000     -1.5308820000
  H4       -1.0828750000      4.7590490000      0.8907050000
  H6       -0.8188550000      2.9597830000      2.5761920000
  C16       0.5634440000     -0.7497030000     -1.1889460000
  C8       -1.4117240000     -1.3116210000      0.3210810000
```

```
  N2       -0.7201180000      0.3261710000      2.1042620000
  C9       -0.7698490000     -1.0448430000      1.6722540000
  C10       0.0413580000      0.6448670000      3.3336860000
  O1       -0.3734810000     -1.9016560000      2.4444420000
  C23      -1.3198870000     -2.7688970000     -0.0904430000
  C18       3.1135660000     -1.4725030000     -2.0799520000
  C19       0.7191740000     -1.5184650000     -2.3463610000
  C20       1.6989500000     -0.3458140000     -0.4858970000
  C21       2.9666510000     -0.7065440000     -0.9292470000
  C22       1.9869010000     -1.8775050000     -2.7877920000
  H2       -0.1643020000     -1.8464500000     -2.9072260000
  H5        1.5937990000      0.2652760000      0.4186800000
  H7        3.8503860000     -0.3855050000     -0.3681160000
  H8        2.0975170000     -2.4806210000     -3.6948610000
  H9        4.1120330000     -1.7559870000     -2.4279520000
  H10      -1.4965740000     -0.4546810000     -1.6459610000
  H19      -0.2770840000     -3.0936510000     -0.2098020000
  H20      -1.8277370000     -2.9334580000     -1.0503940000
  H21      -1.7875140000     -3.4251120000      0.6546050000
  H22      -2.4958910000     -1.0541430000      0.4393710000
  H11       1.1238530000      0.5115470000      3.1939130000
  H12      -0.2877350000     -0.0088720000      4.1524080000
  H13      -0.1482920000      1.6892950000      3.6310450000

  Molecular weight:    251.13 amu

  Stoichiometry:        C17NH17O
  Molecular Point Group: C1
  Point Group used: C1
  nuclear repulsion energy.......  1412.765180051 hartrees

 Non-default options chosen:
   Geometry will be optimized in redundant internal coordinates
   Initial Hessian: from previous calculation

  end of program pre


  start of program onee
  smallest eigenvalue of S:    3.590E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program hfig
  initial wavefunction generated automatically from atomic
wavefunctions

  Irreducible     Total no   No of occupied orbitals
  representation  orbitals   Shell_1  Shell_2    ...
  No Symm          368         67
  ------------------------
```

```
  Orbital occupation/shell    1.000

  end of program hfig


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     89     89     90     89     89     89
81
  grid # 2      116     96     96    100     97     97     99
90
  grid # 3      216    184    184    194    185    185    188
176
  grid # 4      224    326    329    341    327    327    328
308

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     69     91     81     99     84
72
  grid # 2      118    118    109    100     90    108     94
80
  grid # 3      224    224    208    195    176    221    177
150
  grid # 4      232    232    214    339    309    395    300
285

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     72     89     88     88     89     88
70
  grid # 2      122     80     97     95     95     97     96
112
  grid # 3      259    152    184    184    183    184    184
214
  grid # 4      452    295    327    327    328    327    327
220

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       68     73     73     73     66     71     71
71
```

```
  grid # 2      109    118    118    118    107    110    109
110
  grid # 3      208    224    224    224    204    216    215
219
  grid # 4      215    232    232    232    202    218    220
225

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     72     71     69   2872
  grid # 2      113    111    111    105   3741
  grid # 3      220    218    217    204   7224
  grid # 4      217    223    224    209  10068

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf
 number of electrons.........        134
 number of alpha electrons....         67
 number of beta electrons.....         67
 number of orbitals, total....        368
 number of core orbitals......         67
 number of open shell orbs....          0
 number of occupied orbitals..         67
 number of virtual orbitals...        301
 number of hamiltonians.......          1
 number of shells.............          1
 SCF type: HF

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                              energy  density   DIIS
       e  d  i  u  i                 total energy change  change    error

etot   1  N  N  5  M  -780.41271202123          4.7E-03  9.3E-02
etot   2  Y  Y  6  M  -782.69608359237  2.3E+00  1.9E-03  4.4E-02
etot   3  Y  Y  6  M  -782.93430605039  2.4E-01  8.9E-04  2.6E-02
etot   4  N  Y  2  U  -782.99418281974  6.0E-02  8.2E-04  1.6E-02
etot   5  Y  Y  6  M  -783.00512732567  1.1E-02  1.4E-03  9.4E-03
etot   6  N  Y  2  U  -783.01159329142  6.5E-03  1.6E-04  2.0E-03
etot   7  Y  Y  6  M  -783.01198514407  3.9E-04  6.0E-05  5.4E-04
etot   8  Y  Y  6  M  -783.01205427891  6.9E-05  1.3E-05  1.7E-04
etot   9  N  Y  2  U  -783.01192756053 -1.3E-04  5.3E-06  4.2E-05
etot  10  Y  Y  6  M  -783.01193574306  8.2E-06  2.9E-06  2.4E-05
etot  11  Y  N  6  M  -783.01193992884  4.2E-06  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1412.76518005059
   (E)  Total one-electron terms..... -3870.21884252928
   (I)  Total two-electron terms.....  1674.44172254984
   (L)  Electronic energy............. -2195.77711997944  (E+I)
   (N)  Total energy.................  -783.01193992884  (A+L)

 SCFE: SCF energy: HF    -783.01193992884 hartrees   iterations:
11


 HOMO energy:    -0.30125
 LUMO energy:     0.12625

  Orbital energies:
 -20.53715  -15.59909  -11.35721  -11.28812  -11.26378  -11.25438
 -11.25362  -11.24377  -11.24286  -11.24221  -11.24173  -11.23943
 -11.23718  -11.23677  -11.23557  -11.23461  -11.23412  -11.23363
 -11.21757   -1.38363   -1.24570   -1.16565   -1.14286   -1.10822
  -1.03202   -1.01568   -1.01240   -1.00827   -0.94897   -0.93014
  -0.85716   -0.83123   -0.82548   -0.81905   -0.79215   -0.72822
  -0.70806   -0.68929   -0.66805   -0.65889   -0.63944   -0.63211
  -0.62302   -0.61313   -0.60590   -0.60366   -0.59695   -0.58144
  -0.57639   -0.55035   -0.53601   -0.53452   -0.52867   -0.52111
  -0.51144   -0.50619   -0.49768   -0.49477   -0.48448   -0.46783
  -0.46349   -0.42535   -0.40967   -0.34376   -0.33399   -0.32118
  -0.30125    0.12625    0.13182    0.13657    0.14950    0.18956
   0.22736    0.23102    0.23779    0.26005    0.27180

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x             y             z
 ----  -----   -------------  -------------  -------------
   1    H1      9.141887E-04   2.298202E-03   1.437104E-02
   2    C1     -2.767182E-04   3.821136E-03   3.637123E-04
   3    C2      1.602665E-03   1.032900E-03   9.262003E-03
   4    C3     -5.409467E-03   1.377103E-02   3.226114E-03
   5    C4     -1.007726E-03   7.572350E-03  -8.943005E-03
   6    C5      5.966656E-04   5.965702E-03   1.579140E-03
```

```
 7    C6     -7.512541E-03  -4.946018E-03   7.824976E-03
 8    C7     -1.829088E-02  -1.149864E-05  -1.165583E-02
 9    H3      1.306336E-03  -9.881194E-03   9.265149E-03
10    H4      6.785923E-04  -1.336577E-02  -3.689741E-03
11    H6     -4.773891E-03  -8.074146E-04  -2.377465E-02
12    C16     9.177777E-03  -4.456916E-03  -9.468560E-03
13    C8     -1.642419E-02   3.417156E-03   2.538700E-03
14    N2      1.081167E-02  -1.241838E-02  -3.089793E-02
15    C9      1.635634E-02   8.125892E-03   5.980866E-02
16    C10    -5.338862E-03  -4.882477E-03   6.973196E-03
17    O1     -1.643865E-02   2.684856E-02  -3.694026E-02
18    C23     2.996118E-03  -2.064770E-02   2.453127E-03
19    C18     8.026181E-03  -2.386996E-03  -2.887064E-03
20    C19    -1.036851E-03  -9.535367E-04  -2.613440E-03
21    C20     2.783582E-04   3.253334E-03   6.366490E-03
22    C21     6.232964E-03   1.641044E-03   4.793495E-03
23    C22     1.063237E-03  -5.212827E-03  -7.267717E-03
24    H2      1.181075E-02   5.187263E-03   7.186367E-03
25    H5      2.762538E-03  -8.464842E-03  -1.403274E-02
26    H7     -1.104413E-02  -3.889989E-03  -6.993028E-03
27    H8     -1.291282E-03   7.468593E-03   1.101794E-02
28    H9     -1.232420E-02   3.703166E-03   4.203826E-03
29    H10     1.352608E-02   1.291499E-03   1.878991E-02
30    H19    -1.124416E-02   3.527147E-03   2.918004E-03
31    H20     2.955092E-03   3.331649E-03   7.698779E-03
32    H21     4.082163E-03   6.890099E-03  -6.069348E-03
33    H22     1.990731E-02  -9.912844E-04  -4.465324E-04
34    H11    -9.733311E-03   4.534346E-04  -3.985026E-04
35    H12     3.644158E-03   6.090598E-03  -1.193057E-02
36    H13     3.356029E-03  -2.116189E-02  -3.614611E-03
-----------   ------------  ------------  ------------
   total      -6.163477E-05   1.212026E-03  -9.829191E-04

 end of program der1b


 start of program geopt   1

 geometry optimization step  1
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3009844
  Cos(theta):   0.7576404

  Final level shift:  -5.5958388E-02

 gradient maximum:        5.3766E-02 .  (  4.5000E-04 )
 gradient rms:            1.1859E-02 .  (  3.0000E-04 )
 step size:   0.30096  trust radius:   0.30000
```

```
  displacement maximum:    9.1282E-02 .  (  1.8000E-03 )
  displacement rms:        2.7248E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.7469E-02    geom step:   3.0096E-
01    full step:   3.0096E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     2.3725E-02     y:     1.0467E-02     z:    -2.0308E-02

  new geometry:
                                 angstroms
  atom           x                  y                  z
  H1       -1.1044073130      1.8713330404     -2.2243375608
  C1       -1.0564691793      2.1111638591     -1.1743764605
  C2       -0.9343062977      2.7085598799      1.5064722905
  C3       -0.8945234637      1.0769838732     -0.2611975240
  C4       -1.1520226124      3.4316031757     -0.7754905648
  C5       -1.0938470655      3.7211010382      0.5755060778
  C6       -0.8204327992      1.3750850041      1.1016212372
  C7       -0.8059498557     -0.3549639329     -0.7486857811
  H3       -1.2770658291      4.2140759379     -1.5034719232
  H4       -1.1765915218      4.7418251730      0.9115852278
  H6       -0.9115955263      2.9749420037      2.5425376593
  C16       0.5941884749     -0.7498371683     -1.2071061919
  C8       -1.3947650216     -1.2763832191      0.3432281506
  N2       -0.6677369204      0.3271469044      2.0551296154
  C9       -0.7278054746     -1.0116525274      1.6861171244
  C10       0.0022165691      0.5783951795      3.3397709721
  O1       -0.3634093512     -1.8970430890      2.4023312325
  C23      -1.3868687925     -2.7614078637      0.0010427935
  C18       3.1417425411     -1.5171580064     -2.0945587590
  C19       0.7525738427     -1.5293553545     -2.3548028060
  C20       1.7398017891     -0.3500550504     -0.5153615120
  C21       3.0022233054     -0.7308772257     -0.9514072119
  C22       2.0085137154     -1.9143128599     -2.7967410004
  H2       -0.1154452680     -1.8397270774     -2.9142587637
  H5        1.6588842007      0.2513394486      0.3716041259
  H7        3.8724547532     -0.4280729526     -0.3956238749
  H8        2.1071676369     -2.5181807822     -3.6906214644
  H9        4.1176212054     -1.8136960776     -2.4382757552
  H10      -1.4602749474     -0.4516495797     -1.6084472512
  H19      -0.3760732710     -3.1348526160     -0.1136929194
  H20      -1.9304140702     -2.9194034975     -0.9329190712
  H21      -1.8768935520     -3.3371040568      0.7762724172
  H22      -2.4369050182     -0.9742771518      0.4751987922
  H11       1.0870060763      0.5758183343      3.2367673367
  H12      -0.2592759759     -0.1819667151      4.0554160271
  H13      -0.3132843899      1.5332050135      3.7076514697

  nuclear repulsion energy.......  1414.123868993 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   1   /
```

```
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.373E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     87     90     89     89     87
81
  grid # 2      116     96     96    100     97     97     98
90
  grid # 3      216    183    184    194    183    184    187
177
  grid # 4      216    326    330    338    328    328    328
311

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     72     92     81     98     83
70
  grid # 2      118    118    109    100     90    107     91
78
  grid # 3      223    223    207    194    172    215    175
149
  grid # 4      224    223    208    342    315    391    295
272

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     71     89     88     87     89     89
71
  grid # 2      122     79     97     95     96     97     96
112
  grid # 3      259    152    185    183    183    184    184
213
  grid # 4      451    290    330    326    327    329    328
211
```

```
  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       70     73     73     73     67     70     71
70
  grid # 2      109    118    118    118    107    108    109
110
  grid # 3      209    223    223    223    203    216    217
218
  grid # 4      206    223    224    224    195    213    218
216

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     72     71     68   2866
  grid # 2      110    110    111    102   3725
  grid # 3      215    219    215    206   7196
  grid # 4      213    222    213    204   9938

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

        i  u  d  i  g                                          RMS    maximum
        t  p  i  c  r                              energy  density   DIIS
        e  d  i  u  i                 total energy change  change    error

etot    1  N  N  2  U  -783.00933310167          3.5E-04  1.3E-02
etot    2  Y  Y  6  M  -783.02598064401  1.7E-02  1.3E-04  3.2E-03
etot    3  N  Y  2  U  -783.02773332114  1.8E-03  4.3E-05  6.9E-04
etot    4  Y  Y  6  M  -783.02788444362  1.5E-04  2.0E-05  3.1E-04
etot    5  Y  Y  6  M  -783.02790973935  2.5E-05  6.5E-06  1.2E-04
etot    6  Y  Y  6  M  -783.02791817692  8.4E-06  2.7E-06  3.9E-05
etot    7  Y  N  6  M  -783.02791924273  1.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1414.12386899302
   (E)  Total one-electron terms..... -3872.85319047084
   (I)  Total two-electron terms.....  1675.70140223508
   (L)  Electronic energy..... -2197.15178823576  (E+I)
   (N)  Total energy.................  -783.02791924273  (A+L)

 SCFE: SCF energy: HF    -783.02791924273 hartrees   iterations:
7
```

```
HOMO energy:    -0.30333
LUMO energy:     0.12836

 Orbital energies:
 -20.53185  -15.59935  -11.34581  -11.28966  -11.25635  -11.25019
 -11.24230  -11.24206  -11.24139  -11.23921  -11.23800  -11.23629
 -11.23334  -11.23266  -11.23124  -11.23074  -11.23014  -11.23000
 -11.20932   -1.39882   -1.26220   -1.16381   -1.14742   -1.10460
  -1.02970   -1.01808   -1.01564   -1.01219   -0.95770   -0.93204
  -0.85651   -0.83579   -0.83231   -0.82125   -0.79574   -0.73755
  -0.71018   -0.69332   -0.67319   -0.66307   -0.64039   -0.63870
  -0.62778   -0.61496   -0.61027   -0.60855   -0.59571   -0.58358
  -0.57587   -0.55544   -0.54868   -0.53657   -0.53128   -0.51815
  -0.51506   -0.50631   -0.49934   -0.49767   -0.48505   -0.46785
  -0.46297   -0.42636   -0.40832   -0.34266   -0.33260   -0.32075
  -0.30333    0.12836    0.13358    0.14092    0.15021    0.20190
   0.23425    0.23735    0.24341    0.26405    0.27937

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  14    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H1      1.946087E-04  -6.323394E-04   1.067073E-03
  2    C1     -3.357335E-04   5.259749E-04  -1.102102E-03
  3    C2      5.286516E-05  -1.451809E-03  -2.294989E-03
  4    C3      7.209668E-04   2.728785E-03  -1.559457E-03
  5    C4     -2.422060E-04  -1.457961E-03  -8.168008E-04
  6    C5      5.954760E-04   3.916495E-04   1.242561E-03
  7    C6     -4.780141E-03  -1.330682E-03   3.085589E-03
  8    C7     -2.056778E-03  -2.588011E-03   2.251098E-03
  9    H3      2.055660E-04  -5.001011E-04   5.343116E-04
 10    H4      9.717135E-05  -1.729989E-03   5.532171E-04
 11    H6      1.362579E-04  -4.194049E-04   1.212883E-03
 12    C16     5.655386E-03   3.360824E-04  -2.207082E-03
 13    C8     -9.681865E-04  -1.058996E-03   3.247893E-03
 14    N2      1.395083E-02  -1.244992E-02   5.072557E-03
```

```
  15    C9     -1.151127E-02   9.033872E-03  -6.763898E-03
  16    C10     7.216619E-04   2.288058E-03  -7.039939E-03
  17    O1      2.921105E-03   4.592952E-03   3.210847E-03
  18    C23    -8.315517E-04  -6.780812E-04  -4.681604E-03
  19    C18    -4.456733E-03   2.509035E-03   2.491796E-03
  20    C19    -1.131771E-03   1.977221E-03   1.815298E-03
  21    C20     9.283051E-04  -4.855396E-03  -3.169261E-03
  22    C21    -3.162859E-03  -5.768785E-03  -5.785207E-03
  23    C22     5.251910E-03   8.490794E-04   8.132036E-04
  24    H2      2.784072E-04   7.191179E-04   1.286099E-03
  25    H5     -7.321159E-04   1.014848E-03  -9.816183E-04
  26    H7     -1.036353E-04   5.997502E-04  -5.823325E-04
  27    H8     -7.638392E-04   2.933477E-03   4.504432E-03
  28    H9     -1.014318E-05   4.828876E-04   8.564544E-04
  29    H10     2.769634E-04   6.323669E-04  -6.086040E-04
  30    H19    -1.766919E-03  -5.646867E-04   2.565555E-04
  31    H20     2.849561E-03  -3.010745E-04   2.713736E-03
  32    H21     8.618090E-04   8.786714E-04   2.950647E-04
  33    H22     2.662997E-03   2.102258E-03  -1.956764E-04
  34    H11    -2.515887E-03   9.432685E-04  -1.787281E-03
  35    H12    -3.349230E-03  -1.583293E-03  -2.457370E-03
  36    H13     1.946383E-04   2.889798E-03   5.385236E-03
 -----------   -------------  -------------  -------------
    total      -1.625217E-04   1.058626E-03  -1.373169E-04

  end of program der1b


  start of program geopt   2

  geometry optimization step  2
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3004224
   Cos(theta):   0.4752458

   Final level shift:  -1.0193408E-02

  energy change:          -1.5979E-02 .  (  5.0000E-05 )
  gradient maximum:        1.3883E-02 .  (  4.5000E-04 )
  gradient rms:            3.2740E-03 .  (  3.0000E-04 )
  step size:   0.30032  trust radius:   0.30000
  displacement maximum:    1.4458E-01 .  (  1.8000E-03 )
  displacement rms:        2.7190E-02 .  (  1.2000E-03 )
  predicted energy change:    -3.0411E-03    geom step:   3.0032E-
01    full step:   3.0032E-01
  molecular structure not yet converged...

  center of mass moved by:
```

x: 9.4044E-03 y: -3.6558E-03 z: -5.4897E-03

new geometry:

angstroms

atom	x	y	z
H1	-1.1360697545	1.8742896078	-2.2250669586
C1	-1.0840188615	2.1151581333	-1.1805154533
C2	-0.9426935220	2.6908318472	1.5051736170
C3	-0.9005487287	1.0790625100	-0.2757404890
C4	-1.1901160047	3.4300510037	-0.7709666373
C5	-1.1229224671	3.7067201213	0.5834985759
C6	-0.8122468056	1.3664197448	1.0895365823
C7	-0.8035495303	-0.3600011032	-0.7556543070
H3	-1.3305739326	4.2152572254	-1.4881300852
H4	-1.2149035435	4.7166035122	0.9354212552
H6	-0.9195458917	2.9454597831	2.5411422747
C16	0.6065900665	-0.7600676717	-1.1987684706
C8	-1.4218257511	-1.2550847214	0.3443807818
N2	-0.5804256437	0.3168091697	2.0161367163
C9	-0.7372176302	-0.9906914408	1.6733491806
C10	0.0498103660	0.5862375897	3.3046014253
O1	-0.3758180446	-1.8682573311	2.3962863770
C23	-1.4681588409	-2.7467585512	0.0219699547
C18	3.1633959297	-1.5162621679	-2.0721964362
C19	0.7767763762	-1.5292988058	-2.3491706197
C20	1.7440894845	-0.3807688249	-0.4940736241
C21	3.0067797454	-0.7607484945	-0.9195083335
C22	2.0402485898	-1.9013215486	-2.7871331595
H2	-0.0857552719	-1.8383658836	-2.9087742654
H5	1.6560392450	0.2289821634	0.3860345867
H7	3.8680007309	-0.4549663862	-0.3526674223
H8	2.1441734788	-2.4771717074	-3.6886626114
H9	4.1426390988	-1.7957748570	-2.4096253936
H10	-1.4347344162	-0.4605117222	-1.6254863459
H19	-0.4768013365	-3.1680587561	-0.0702709643
H20	-1.9992991883	-2.8990580916	-0.9100200157
H21	-1.9899128036	-3.2866754663	0.8024066192
H22	-2.4394701476	-0.8910029944	0.4718169078
H11	1.1210176656	0.7873111837	3.1580355925
H12	-0.0602355674	-0.2910893768	3.9457674038
H13	-0.4238431094	1.4429866643	3.7983296778

nuclear repulsion energy..... 1416.623512852 hartrees

/ end of geometry optimization iteration 2 /

end of program geopt

start of program onee
smallest eigenvalue of S: 3.329E-04

```
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     87     90     89     87     84
82
  grid # 2      116     96     96     98     97     97     94
90
  grid # 3      215    182    184    196    183    184    189
174
  grid # 4      216    326    329    339    329    328    325
309

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     72     92     82     97     82
70
  grid # 2      118    118    110    100     91    105     92
79
  grid # 3      224    223    208    197    175    211    175
149
  grid # 4      224    223    208    339    309    387    291
280

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     87     89     89
71
  grid # 2      122     80     97     95     96     97     96
112
  grid # 3      256    150    184    183    182    184    183
213
  grid # 4      451    285    327    326    327    328    329
212

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       69     73     73     73     67     70     71
70
```

```
  grid # 2      109    118    118    118    108    108    110
110
  grid # 3      209    223    223    224    203    218    218
218
  grid # 4      205    223    224    224    197    213    216
217

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       68     72     70     69   2862
  grid # 2      110    110    109    104   3724
  grid # 3      213    218    212    212   7195
  grid # 4      212    222    216    217   9933

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

        i  u  d  i  g
        t  p  i  c  r                                  RMS    maximum
        e  d  i  u  i                      energy  density   DIIS
        r  t  s  t  d     total energy     change  change    error

etot    1  N  N  2  U  -783.01126167785           3.3E-04  1.0E-02
etot    2  Y  Y  6  M  -783.02756536761  1.6E-02  1.4E-04  2.3E-03
etot    3  N  Y  2  U  -783.02941461835  1.8E-03  3.7E-05  5.9E-04
etot    4  Y  Y  6  M  -783.02952980645  1.2E-04  2.0E-05  3.9E-04
etot    5  Y  Y  6  M  -783.02955569322  2.6E-05  5.6E-06  1.3E-04
etot    6  Y  Y  6  M  -783.02955625824  5.7E-07  3.9E-06  7.7E-05
etot    7  Y  N  6  M  -783.02955823967  2.0E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1416.62351285185
   (E)  Total one-electron terms..... -3877.84708094885
   (I)  Total two-electron terms.....  1678.19400985733
   (L)  Electronic energy............. -2199.65307109152  (E+I)
   (N)  Total energy.................  -783.02955823967  (A+L)

 SCFE: SCF energy: HF    -783.02955823967 hartrees   iterations:
7


 HOMO energy:    -0.30329
 LUMO energy:     0.12886

  Orbital energies:
```

```
 -20.52393  -15.59890  -11.34104  -11.28808  -11.26075  -11.25040
 -11.24254  -11.24157  -11.24091  -11.23846  -11.23747  -11.23532
 -11.23132  -11.23028  -11.23027  -11.22980  -11.22842  -11.22766
 -11.20910   -1.40050   -1.26814   -1.16465   -1.14898   -1.10534
  -1.02968   -1.01982   -1.01688   -1.01217   -0.95912   -0.93297
  -0.85644   -0.83983   -0.83320   -0.82166   -0.79562   -0.74108
  -0.71109   -0.69488   -0.67387   -0.66454   -0.64360   -0.63853
  -0.62759   -0.61470   -0.60960   -0.60823   -0.59616   -0.58286
  -0.57644   -0.55375   -0.54498   -0.53824   -0.53275   -0.51810
  -0.51548   -0.50705   -0.50060   -0.49713   -0.48496   -0.46759
  -0.46327   -0.42315   -0.40789   -0.34270   -0.33191   -0.32224
  -0.30329    0.12886    0.13437    0.14322    0.15119    0.20670
   0.23147    0.23934    0.24427    0.26230    0.28157

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
   1    H1     -3.082926E-04  -3.577662E-04  -2.723169E-03
   2    C1     -1.374969E-04  -2.418166E-03   1.456064E-03
   3    C2      1.377452E-05  -1.975922E-03  -2.303282E-03
   4    C3      2.018110E-03  -7.466640E-04  -1.121869E-03
   5    C4      2.855550E-05  -1.102416E-03   3.136204E-03
   6    C5     -2.056760E-04  -7.299525E-04  -1.059909E-03
   7    C6     -1.443225E-03   2.149661E-04  -7.743155E-04
   8    C7      3.076217E-03   2.254134E-04   3.074695E-03
   9    H3     -2.907090E-06   1.426743E-03  -1.108113E-03
  10    H4     -3.322195E-04   1.814071E-03   5.214524E-04
  11    H6      1.396287E-03   3.418925E-04   3.663329E-03
  12    C16    -2.764643E-04  -1.974808E-03  -9.513047E-04
  13    C8      2.386595E-03   5.808208E-05  -4.735133E-05
  14    N2     -8.230422E-04   1.301818E-02   3.454141E-03
  15    C9     -3.058066E-03  -3.232140E-03  -8.598742E-03
  16    C10     3.755395E-03   3.830755E-03   7.517243E-03
  17    O1      1.526089E-03  -1.246560E-02   6.372886E-03
  18    C23    -5.343014E-04   2.435888E-03   1.210217E-03
  19    C18    -3.585844E-03   7.361023E-04   1.488049E-03
  20    C19     1.774767E-03   1.741698E-03   2.546390E-03
  21    C20     1.244480E-03   3.080191E-04   3.133983E-04
```

```
 22    C21    -2.899414E-04  -2.262326E-04  -1.249966E-03
 23    C22    -1.044410E-03   2.231700E-03   1.966240E-03
 24    H2     -1.867735E-03  -2.905530E-04  -1.773009E-03
 25    H5     -1.970375E-04  -9.438230E-05   1.993314E-05
 26    H7      5.917706E-04   9.230519E-05  -6.502731E-05
 27    H8     -7.554945E-05  -1.095927E-03  -4.333006E-04
 28    H9      2.087984E-03  -7.024403E-04  -4.409341E-04
 29    H10    -3.074972E-03   2.599989E-04  -2.740369E-03
 30    H19     7.075277E-04   1.957997E-04   1.500077E-04
 31    H20    -5.889766E-04  -7.818218E-04  -1.992273E-03
 32    H21     6.018829E-04   4.955222E-04   6.605755E-05
 33    H22    -1.584246E-03  -4.799049E-04  -3.840279E-04
 34    H11    -9.062111E-03   4.534365E-04   4.164608E-03
 35    H12     1.032214E-03   9.121153E-03  -8.381801E-03
 36    H13     5.812112E-03  -9.340463E-03  -5.088915E-03
-----------   -------------  -------------  -------------
   total      -4.387537E-04   9.865719E-04  -1.167636E-04

 end of program der1b


 start of program geopt   3

 geometry optimization step  3
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3000187
  Cos(theta):   0.4304456

  Final level shift:  -2.3415623E-02

 energy change:          -1.6390E-03 .  (  5.0000E-05 )
 gradient maximum:        1.6008E-02 .  (  4.5000E-04 )
 gradient rms:            3.3268E-03 .  (  3.0000E-04 )
 step size:   0.30001  trust radius:   0.30000
 displacement maximum:    1.4189E-01 .  (  1.8000E-03 )
 displacement rms:        2.7162E-02 .  (  1.2000E-03 )
 predicted energy change:    -3.4265E-03    geom step:   3.0001E-
01    full step:   3.0001E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:    -5.9121E-03     y:    -8.8655E-04     z:     2.9321E-03

 new geometry:
                                angstroms
 atom            x                  y                  z
```

```
 H1       -1.1493192298      1.8549570154     -2.2333524104
 C1       -1.0889707199      2.1012066989     -1.1879689517
 C2       -0.9198667501      2.6769792995      1.5030431629
 C3       -0.8960253495      1.0688914711     -0.2816578291
 C4       -1.1918953639      3.4154289299     -0.7687059651
 C5       -1.1081724709      3.6941058353      0.5863385034
 C6       -0.7993553177      1.3562670778      1.0844000074
 C7       -0.8032988283     -0.3721428087     -0.7535023231
 H3       -1.3375010225      4.2061158093     -1.4826277171
 H4       -1.1944911019      4.7020547520      0.9481100929
 H6       -0.8713806391      2.9235448060      2.5484031802
 C16       0.6105468049     -0.7661182892     -1.1944206999
 C8       -1.4370684163     -1.2566808480      0.3430664849
 N2       -0.5609220548      0.3171850594      2.0090130115
 C9       -0.7733402972     -0.9795796976      1.6704048202
 C10       0.0600028007      0.5985285071      3.2910755977
 O1       -0.4197465597     -1.8409690317      2.4296367502
 C23      -1.4570554976     -2.7454651033      0.0209145727
 C18       3.1631594968     -1.5012243862     -2.0755987501
 C19       0.7768837493     -1.5234106775     -2.3482403375
 C20       1.7460687721     -0.3888219979     -0.4919430700
 C21       3.0048742457     -0.7613909560     -0.9227307771
 C22       2.0444150447     -1.8822940505     -2.7876195566
 H2       -0.0912186844     -1.8350218347     -2.9032575625
 H5        1.6490696112      0.2436445877      0.3783725401
 H7        3.8693043640     -0.4359582748     -0.3622568289
 H8        2.1462113417     -2.4509827533     -3.6892265640
 H9        4.1495791890     -1.7709647155     -2.4122289481
 H10      -1.4319212987     -0.4663217436     -1.6368910492
 H19      -0.4600411396     -3.1610622982     -0.0378645957
 H20      -1.9434613706     -2.9178713257     -0.9266809129
 H21      -1.9884094504     -3.2866763685      0.7966882395
 H22      -2.4517128350     -0.8800950580      0.4457908417
 H11       1.0759014206      0.6927316915      3.1964041677
 H12      -0.1529860282     -0.1870859035      3.9118585895
 H13      -0.2863540708      1.4456298553      3.7688514561

 nuclear repulsion energy.......  1419.539075954 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   3   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.329E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
```

```
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     88     90     89     87     85
82
  grid # 2      116     96     96     98     97     97     93
90
  grid # 3      217    180    184    196    184    184    193
175
  grid # 4      216    327    328    337    328    329    325
310

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     72     92     82     97     82
67
  grid # 2      118    118    110    100     90    106     91
76
  grid # 3      224    223    209    196    172    211    174
136
  grid # 4      224    223    209    339    313    388    294
263

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     71     89     88     87     88     88
71
  grid # 2      122     79     97     95     96     97     96
112
  grid # 3      258    154    183    183    182    182    182
213
  grid # 4      451    286    327    326    330    330    327
212

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       70     73     73     73     68     70     71
70
  grid # 2      109    118    118    118    107    110    108
108
  grid # 3      209    223    223    223    202    216    216
219
  grid # 4      205    223    223    224    200    212    213
218
```

```
  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       68     70     69     68   2854
  grid # 2      111    109    107    104   3713
  grid # 3      215    212    206    203   7162
  grid # 4      212    213    210    206   9901

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy       change  change    error

etot   1  N  N  2  U  -783.01302857733                2.3E-04  5.8E-03
etot   2  Y  Y  6  M  -783.02012638625  7.1E-03       7.9E-05  1.4E-03
etot   3  N  Y  2  U  -783.02079516149  6.7E-04       3.1E-05  5.5E-04
etot   4  Y  Y  6  M  -783.02088495478  9.0E-05       1.2E-05  2.2E-04
etot   5  Y  Y  6  M  -783.02089763379  1.3E-05       5.6E-06  1.1E-04
etot   6  Y  Y  6  M  -783.02089777146  1.4E-07       2.2E-06  4.0E-05
etot   7  Y  N  6  M  -783.02089839267  6.2E-07       0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1419.53907595437
   (E)  Total one-electron terms..... -3883.59564636171
   (I)  Total two-electron terms.....  1681.03567201467
   (L)  Electronic energy............. -2202.55997434705  (E+I)
   (N)  Total energy.................  -783.02089839267  (A+L)

 SCFE: SCF energy: HF    -783.02089839267 hartrees   iterations:
7


 HOMO energy:    -0.30130
 LUMO energy:     0.12937

  Orbital energies:
  -20.52047  -15.59739  -11.34077  -11.28493  -11.25105  -11.24365
  -11.24140  -11.23981  -11.23808  -11.23773  -11.23666  -11.23413
  -11.23050  -11.23034  -11.22951  -11.22925  -11.22744  -11.22697
  -11.20981   -1.39598   -1.26875   -1.16619   -1.14939   -1.10795
   -1.03141   -1.02051   -1.01889   -1.01252   -0.97489   -0.93373
   -0.86150   -0.84070   -0.83382   -0.82162   -0.79707   -0.74148
```

```
 -0.71445   -0.69607   -0.67339   -0.66638   -0.64892   -0.64008
 -0.62724   -0.61523   -0.61465   -0.60687   -0.60107   -0.58268
 -0.57697   -0.55583   -0.54910   -0.54255   -0.53442   -0.52076
 -0.51394   -0.50947   -0.50162   -0.49716   -0.48439   -0.46724
 -0.46323   -0.42313   -0.40901   -0.34306   -0.33238   -0.32328
 -0.30130    0.12937    0.13491    0.14364    0.15253    0.20638
  0.23329    0.23913    0.24748    0.26358    0.28257

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -3.568831E-04   1.109415E-03  -9.209897E-04
  2    C1     -2.034352E-05  -1.371284E-03   3.412681E-03
  3    C2      6.594593E-04   8.082592E-04   3.460529E-03
  4    C3      7.149387E-04  -1.108120E-03  -2.771394E-05
  5    C4      4.143396E-05   1.674032E-03   1.156189E-03
  6    C5     -6.124662E-04  -7.993811E-04  -2.016390E-03
  7    C6     -9.979712E-04   3.541656E-03  -4.343465E-03
  8    C7      1.651353E-03   4.281931E-03  -3.413555E-03
  9    H3      2.770288E-05  -6.347445E-06  -5.799076E-05
 10    H4     -2.518476E-04   1.548362E-03  -1.172001E-03
 11    H6      1.090440E-06   5.570033E-05  -2.801159E-03
 12    C16    -5.590590E-03  -2.884466E-03   1.078663E-04
 13    C8      3.901099E-03   2.198532E-03  -4.843406E-03
 14    N2     -9.004261E-03   2.417988E-02  -9.148776E-03
 15    C9      1.316206E-02  -1.263653E-02   1.555977E-02
 16    C10    -2.091783E-02  -8.387531E-03  -2.588062E-02
 17    O1     -6.362973E-03  -1.077377E-02  -5.313159E-03
 18    C23     1.064210E-05  -1.697078E-03   7.251403E-03
 19    C18     3.920470E-03  -2.525265E-03  -1.577304E-03
 20    C19     2.348930E-03  -5.013517E-04   8.022096E-04
 21    C20    -1.561557E-03   6.977441E-03   5.496451E-03
 22    C21     5.480977E-03   6.943500E-03   6.945698E-03
 23    C22    -6.692890E-03  -4.001955E-04  -1.293996E-03
 24    H2      6.932007E-04   1.607263E-04  -1.484115E-03
 25    H5      1.565549E-03  -4.176075E-03  -2.465750E-03
 26    H7     -2.106746E-03  -1.924741E-03  -1.496112E-03
 27    H8      6.593698E-04  -2.594396E-03  -3.254325E-03
```

```
 28    H9     -9.790639E-04  -3.527771E-04  -5.421059E-04
 29    H10     2.372693E-04  -2.426165E-04   2.689595E-03
 30    H19     1.136903E-03   1.805316E-03   9.194666E-04
 31    H20    -3.754292E-03  -1.069086E-04  -3.654333E-03
 32    H21     1.202550E-04   2.585181E-04  -2.077064E-03
 33    H22    -3.077850E-03  -2.638022E-03  -4.479005E-05
 34    H11     5.095475E-02   2.735351E-03  -6.412508E-03
 35    H12    -5.699583E-03  -3.713791E-02   2.700621E-02
 36    H13    -2.016409E-02   3.468502E-02   8.876179E-03
-----------   -------------  -------------  -------------
   total      -8.637910E-04   6.988612E-04  -5.573905E-04

 end of program der1b


 start of program geopt   4

 geometry optimization step  4
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 ** restarting optimization from step    3 **


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3000088
  Cos(theta):   0.3468320

  Final level shift:  -4.6477544E-03

 energy change:           8.6598E-03 .  (  5.0000E-05 )
 gradient maximum:        1.6008E-02 .  (  4.5000E-04 )
 gradient rms:            3.3268E-03 .  (  3.0000E-04 )
 step size:   0.30000  trust radius:   0.30000
 displacement maximum:    2.0871E-01 .  (  1.8000E-03 )
 displacement rms:        2.7161E-02 .  (  1.2000E-03 )
 predicted energy change:    -2.1209E-03    geom step:   3.0000E-
01    full step:   3.0000E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:     3.0531E-16     y:     2.5674E-16     z:     1.8041E-16

 new geometry:
                                angstroms
 atom            x                  y                  z
 H1       -1.1633551772      1.8563015717     -2.2324942395
 C1       -1.1020801029      2.1011419220     -1.1855337355
 C2       -0.9333770541      2.6928815163      1.4963997947
 C3       -0.9068984257      1.0743675058     -0.2756730726
 C4       -1.2089092658      3.4181926731     -0.7748811645
```

```
 C5       -1.1258719877      3.7062674442      0.5748592748
 C6       -0.8190090682      1.3702307238      1.0842322605
 C7       -0.8109219429     -0.3637552418     -0.7420620716
 H3       -1.3525432390      4.2035165896     -1.4947385471
 H4       -1.2153541208      4.7187624676      0.9242781490
 H6       -0.8792644236      2.9464446577      2.5369332952
 C16       0.5998135239     -0.7609837907     -1.1844367879
 C8       -1.4346868045     -1.2586593521      0.3496428123
 N2       -0.6015805692      0.3402074299      2.0250700567
 C9       -0.8000852167     -0.9908956640      1.6976321864
 C10       0.1000734513      0.6280608397      3.2573210571
 O1       -0.5241894247     -1.8818723679      2.4504411667
 C23      -1.4192955636     -2.7455302146      0.0269498146
 C18       3.1453393606     -1.5322304049     -2.0545929201
 C19       0.7678565424     -1.4549760980     -2.3759341694
 C20       1.7347899681     -0.4537889460     -0.4360001075
 C21       2.9933213824     -0.8374564436     -0.8641945107
 C22       2.0277697011     -1.8396421344     -2.8090340544
 H2       -0.0925439642     -1.7059342518     -2.9732360828
 H5        1.6392195545      0.0976658034      0.4776029570
 H7        3.8547949909     -0.5851437026     -0.2716841929
 H8        2.1297572060     -2.3817742564     -3.7353353249
 H9        4.1255838386     -1.8263465003     -2.3888709798
 H10      -1.4531206240     -0.4589074672     -1.6138996699
 H19      -0.4105096091     -3.1316235194     -0.0022191808
 H20      -1.8804521048     -2.9211740423     -0.9393326761
 H21      -1.9570009496     -3.2972648333      0.7853575737
 H22      -2.4613718355     -0.9263682900      0.4438689715
 H11       1.1105134807      0.9761402849      3.0595440790
 H12       0.1347721393     -0.2860870124      3.8277845169
 H13      -0.4423094524      1.3804770232      3.8276914395

 nuclear repulsion energy.......  1417.707311794 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   4   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.296E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe


 start of program grid
```

number of gridpoints:

atom	H1	C1	C2	C3	C4	C5	C6	C7
grid # 1	72	87	87	90	89	87	84	82
grid # 2	116	97	96	99	97	97	94	90
grid # 3	217	182	183	194	184	183	185	175
grid # 4	216	326	328	338	328	328	324	312

number of gridpoints:

atom	H3	H4	H6	C16	C8	N2	C9	C10
grid # 1	73	73	71	92	82	97	82	69
grid # 2	118	118	109	100	90	107	91	79
grid # 3	224	223	207	193	173	214	176	142
grid # 4	224	223	207	340	310	391	294	275

number of gridpoints:

atom	O1	C23	C18	C19	C20	C21	C22	H2
grid # 1	111	73	89	88	88	89	89	71
grid # 2	122	80	97	95	96	97	96	112
grid # 3	256	148	183	182	183	184	183	212
grid # 4	448	287	327	326	327	327	327	211

number of gridpoints:

atom	H5	H7	H8	H9	H10	H19	H20	H21
grid # 1	70	73	73	73	68	70	72	70
grid # 2	110	118	118	118	106	108	108	108
grid # 3	210	223	223	224	200	218	216	217
grid # 4	205	223	223	224	200	210	215	216

number of gridpoints:

atom	H22	H11	H12	H13	total
grid # 1	69	72	70	70	2865
grid # 2	109	111	106	108	3721

```
 grid # 3      215    219    212    212   7175
 grid # 4      209    220    209    216   9914

 end of program grid


 start of program rwr
recomputing RwR matrix  14    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                    energy  density   DIIS
      r  t  s  t  d     total energy    change  change    error

etot  1  N  N  2  U  -782.99741651887           4.2E-04  1.4E-02
etot  2  Y  Y  6  M  -783.02714430037  3.0E-02  1.8E-04  4.6E-03
etot  3  N  Y  2  U  -783.03065471497  3.5E-03  5.2E-05  1.3E-03
etot  4  Y  Y  6  M  -783.03092186826  2.7E-04  2.5E-05  5.7E-04
etot  5  Y  Y  6  M  -783.03096448040  4.3E-05  7.4E-06  1.9E-04
etot  6  Y  Y  6  M  -783.03096754878  3.1E-06  4.0E-06  6.9E-05
etot  7  Y  N  6  M  -783.03096691260 -6.4E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1417.70731179423
   (E)  Total one-electron terms..... -3879.95241723759
   (I)  Total two-electron terms.....  1679.21413853077
   (L)  Electronic energy............. -2200.73827870682  (E+I)
   (N)  Total energy.................  -783.03096691260  (A+L)

 SCFE: SCF energy: HF    -783.03096691260 hartrees   iterations:
7


 HOMO energy:    -0.30305
 LUMO energy:     0.12851

  Orbital energies:
  -20.52924  -15.59861  -11.34677  -11.28442  -11.25553  -11.25004
  -11.24133  -11.24126  -11.24095  -11.23773  -11.23745  -11.23413
  -11.23196  -11.23134  -11.23022  -11.23014  -11.22926  -11.22865
  -11.20814   -1.39823   -1.26965   -1.16595   -1.14955   -1.10730
   -1.03120   -1.01904   -1.01814   -1.01359   -0.96000   -0.93299
   -0.85825   -0.83775   -0.83370   -0.82215   -0.79680   -0.74078
   -0.71277   -0.69485   -0.67459   -0.66504   -0.64292   -0.63990
   -0.62782   -0.61486   -0.61216   -0.61038   -0.59766   -0.58402
   -0.57674   -0.55325   -0.54745   -0.53787   -0.53249   -0.51849
   -0.51597   -0.50798   -0.50078   -0.49866   -0.48579   -0.46821
```

```
  -0.46375   -0.42396   -0.40898   -0.34282   -0.33374   -0.32291
  -0.30305    0.12851    0.13390    0.14322    0.15264    0.20174
   0.22945    0.23975    0.24199    0.26315    0.28317

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  14    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1      1.464204E-05   4.100440E-04   1.429785E-04
  2    C1     -1.934440E-04   6.625458E-04   3.809673E-04
  3    C2      3.553541E-05   2.010971E-03   2.338527E-03
  4    C3     -2.814063E-05  -7.084640E-04  -1.725607E-03
  5    C4      8.937528E-05   5.141429E-04  -1.135960E-03
  6    C5      1.047709E-04  -5.602961E-04   6.674672E-05
  7    C6     -8.830665E-04   1.908109E-03  -1.272690E-03
  8    C7     -1.802835E-04   1.511958E-03  -1.944819E-03
  9    H3     -3.195135E-04   2.547806E-06  -2.444269E-04
 10    H4      1.285197E-04   8.416326E-04  -3.065592E-04
 11    H6      8.829953E-05  -2.086844E-04  -7.799027E-05
 12    C16    -2.037599E-03  -3.708856E-04   1.091438E-03
 13    C8      5.285677E-03   5.334815E-04  -2.661344E-03
 14    N2      1.571448E-03  -1.315674E-02  -8.564086E-03
 15    C9     -3.753237E-04   4.540180E-03   3.982317E-03
 16    C10    -5.036975E-03   2.602461E-03   8.503628E-03
 17    O1      1.244286E-03   3.164417E-03   9.663999E-04
 18    C23    -3.921881E-04  -1.050751E-03   5.379541E-04
 19    C18     1.592684E-03  -2.271867E-04   1.280388E-04
 20    C19     1.142277E-04  -9.305281E-04  -4.444689E-04
 21    C20    -1.585496E-03  -5.574615E-04  -1.865744E-03
 22    C21    -4.057457E-04   3.715028E-04  -4.552219E-04
 23    C22    -3.081876E-04  -1.411942E-03  -1.918443E-03
 24    H2      6.451544E-05   4.770104E-04   1.223478E-04
 25    H5      2.545576E-04   1.175920E-03   1.809985E-03
 26    H7      3.131506E-04  -2.401508E-04   1.654977E-04
 27    H8      1.400414E-04   1.034914E-03   1.143974E-03
 28    H9     -6.033220E-04   7.040285E-05   1.326459E-04
 29    H10     1.651611E-03  -6.505141E-04   6.439674E-04
 30    H19     1.251459E-03   2.207528E-05  -2.259209E-04
```

```
  31    H20    -1.191776E-03  -4.697697E-04  -9.416003E-05
  32    H21    -1.132301E-03  -8.413707E-04  -6.256883E-04
  33    H22    -4.766563E-03   9.381541E-04   3.613748E-04
  34    H11    -1.156986E-03   1.313362E-03   6.536929E-04
  35    H12     1.653617E-03   2.348664E-03   5.855605E-04
  36    H13     4.772054E-03  -3.883262E-03  -1.372253E-04
 ----------   ------------  ------------  ------------
    total      -2.264399E-04   1.186487E-03   5.768563E-05

  end of program der1b


  start of program geopt   5

  geometry optimization step  5
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3001009
   Cos(theta):   0.4486299

   Final level shift:  -4.8335520E-03

  energy change:          -1.4087E-03 .  (  5.0000E-05 )
  gradient maximum:        9.0972E-03 .  (  4.5000E-04 )
  gradient rms:            2.2072E-03 .  (  3.0000E-04 )
  step size:   0.30010  trust radius:   0.30000
  displacement maximum:    2.0592E-01 .  (  1.8000E-03 )
  displacement rms:        2.7170E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.8588E-03    geom step:   3.0010E-
01    full step:   3.0010E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     3.5588E-02     y:    -1.2864E-03     z:    -1.7007E-02

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -1.2175400770      1.8891052826     -2.2177329589
  C1       -1.1314297062      2.1230271475     -1.1714197668
  C2       -0.9028029714      2.6944881803      1.5135553850
  C3       -0.9019009468      1.0878425486     -0.2771188893
  C4       -1.2437519012      3.4374570079     -0.7509859213
  C5       -1.1288300998      3.7125312626      0.6000330470
  C6       -0.7841845123      1.3732251423      1.0876863759
  C7       -0.8052084276     -0.3493133277     -0.7537163719
  H3       -1.4220405433      4.2242805365     -1.4617471887
```

```
 H4       -1.2216472407      4.7226961691      0.9552563440
 H6       -0.8355978117      2.9479178605      2.5491983407
 C16       0.5981943429     -0.7589932800     -1.2028624296
 C8       -1.4200845787     -1.2454522800      0.3459862471
 N2       -0.5278245541      0.3182203051      1.9979875268
 C9       -0.7528996285     -0.9922136686      1.6891804531
 C10      -0.0158299262      0.6023961828      3.3484557402
 O1       -0.4629203846     -1.8791586606      2.4321068004
 C23      -1.4630815373     -2.7381662148      0.0205574768
 C18       3.1405587001     -1.5539040849     -2.0693293663
 C19       0.7572742841     -1.5327935091     -2.3476846321
 C20       1.7420092775     -0.3800780004     -0.5080240027
 C21       2.9977907762     -0.7773104015     -0.9328209995
 C22       2.0134325565     -1.9294715036     -2.7794880433
 H2       -0.1099334243     -1.8292779118     -2.9117304019
 H5        1.6639504359      0.2438317829      0.3630341675
 H7        3.8650378847     -0.4748931292     -0.3751628581
 H8        2.1079595795     -2.5245349356     -3.6681080206
 H9        4.1162528399     -1.8593900805     -2.3972518101
 H10      -1.4431126629     -0.4505981245     -1.6199730510
 H19      -0.4701613873     -3.1364041874     -0.0899990459
 H20      -2.0113224545     -2.9039570150     -0.9004167911
 H21      -1.9598129558     -3.2850251643      0.8051757424
 H22      -2.4445552636     -0.8875109184      0.4634908948
 H11       1.0027822253      0.9879917141      3.2861897984
 H12      -0.0146348396     -0.3081264344      3.9162292564
 H13      -0.6232269453      1.3263127769      3.8768996492

 nuclear repulsion energy.......  1415.176077164 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   5   /
 ------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.339E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H1     C1     C2     C3     C4     C5     C6
C7
```

```
  grid # 1       72     87     87     90     89     87     85
81
  grid # 2      116     96     96     98     97     97     93
90
  grid # 3      216    182    184    196    183    184    195
176
  grid # 4      216    326    329    337    328    328    329
312

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     95     81
71
  grid # 2      118    118    109    100     91    106     92
78
  grid # 3      224    223    207    195    176    211    175
144
  grid # 4      224    223    206    342    311    388    295
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     87     89     89
71
  grid # 2      122     80     97     95     96     97     96
112
  grid # 3      256    144    183    182    182    183    183
212
  grid # 4      451    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     70     71
71
  grid # 2      111    118    118    118    107    108    108
110
  grid # 3      209    222    223    223    202    217    217
218
  grid # 4      205    223    223    224    196    213    218
216

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     72     70     70   2864
  grid # 2      110    112    106    107   3723
  grid # 3      216    219    212    212   7186
  grid # 4      212    223    209    211   9923
```

```
  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                        energy  density   DIIS
      r  t  s  t  d     total energy       change  change    error

etot  1  N  N  2  U  -783.00565528562                3.5E-04  1.3E-02
etot  2  Y  Y  6  M  -783.02800145471  2.2E-02       1.6E-04  5.2E-03
etot  3  N  Y  2  U  -783.03083257570  2.8E-03       4.8E-05  1.4E-03
etot  4  Y  Y  6  M  -783.03098268390  1.5E-04       2.2E-05  5.7E-04
etot  5  Y  Y  6  M  -783.03101801400  3.5E-05       6.6E-06  1.8E-04
etot  6  Y  Y  6  M  -783.03102679647  8.8E-06       3.8E-06  6.0E-05
etot  7  Y  N  6  M  -783.03102700316  2.1E-07       0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.17607716368
   (E)  Total one-electron terms..... -3874.95605560991
   (I)  Total two-electron terms.....  1676.74895144308
   (L)  Electronic energy............. -2198.20710416683  (E+I)
   (N)  Total energy.................  -783.03102700316  (A+L)

 SCFE: SCF energy: HF    -783.03102700316 hartrees   iterations:
7


 HOMO energy:    -0.30253
 LUMO energy:     0.12953

  Orbital energies:
  -20.52568  -15.60100  -11.34352  -11.28825  -11.25769  -11.24950
  -11.24220  -11.24163  -11.23974  -11.23889  -11.23804  -11.23554
  -11.23051  -11.23027  -11.22907  -11.22881  -11.22731  -11.22649
  -11.20732   -1.40061   -1.26749   -1.16444   -1.14866   -1.10494
   -1.02910   -1.01916   -1.01726   -1.01203   -0.96151   -0.93310
   -0.85759   -0.83965   -0.83306   -0.82117   -0.79602   -0.74118
   -0.71093   -0.69471   -0.67347   -0.66385   -0.64386   -0.63756
   -0.62727   -0.61448   -0.61116   -0.60786   -0.59555   -0.58267
   -0.57636   -0.55276   -0.54906   -0.54037   -0.53356   -0.51828
   -0.51470   -0.50688   -0.50069   -0.49741   -0.48420   -0.46856
   -0.46230   -0.42299   -0.40995   -0.34211   -0.33203   -0.32252
   -0.30253    0.12953    0.13450    0.14466    0.15174    0.20709
    0.23131    0.24045    0.24714    0.26252    0.28489
```

```
 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-9.772272E-05	-4.189946E-04	-8.617804E-04
2	C1	2.892658E-04	-1.044628E-03	9.403658E-04
3	C2	-3.852789E-04	-6.887077E-04	-2.366643E-03
4	C3	6.994017E-04	1.156130E-03	-5.214725E-04
5	C4	2.227282E-04	-1.322025E-03	1.865788E-03
6	C5	-7.378215E-05	-1.181298E-03	-9.430545E-04
7	C6	-6.531849E-04	-1.235538E-03	-1.486967E-03
8	C7	1.790404E-03	-1.161458E-03	1.688684E-03
9	H3	1.791568E-04	-1.137047E-05	1.725852E-04
10	H4	1.315490E-04	6.488483E-04	5.624561E-04
11	H6	1.301057E-03	-3.265359E-04	3.037153E-03
12	C16	7.609630E-05	1.061713E-03	5.856959E-04
13	C8	-1.713497E-03	-1.298434E-03	-7.510117E-05
14	N2	3.187611E-04	1.143298E-02	1.677951E-02
15	C9	-3.001685E-03	4.365987E-04	-1.424916E-02
16	C10	5.239394E-03	5.428258E-03	-7.204355E-03
17	O1	9.472003E-04	-9.054205E-03	7.952017E-03
18	C23	-1.913171E-03	5.482054E-03	-1.191674E-03
19	C18	-8.034273E-04	-8.017305E-04	-5.108291E-04
20	C19	-8.529842E-04	-2.264568E-04	-2.443258E-04
21	C20	5.536663E-04	1.326195E-03	1.300569E-03
22	C21	4.955351E-06	2.285444E-04	5.610014E-04
23	C22	-6.142856E-04	1.113482E-03	1.248098E-03
24	H2	-5.417473E-04	-1.940381E-04	-2.996522E-04
25	H5	-4.606561E-04	-4.813773E-04	1.537452E-04
26	H7	9.641438E-04	4.738561E-04	5.131780E-04
27	H8	5.102141E-05	-1.088101E-03	-1.475104E-03
28	H9	1.429508E-03	-3.948510E-04	-7.109323E-04
29	H10	-2.406398E-03	1.854263E-04	-2.272604E-03
30	H19	4.092032E-03	-2.740082E-03	-5.014442E-04
31	H20	2.337552E-04	5.880185E-04	-1.844656E-03
32	H21	-7.434519E-04	-7.530827E-04	3.108658E-03
33	H22	4.976110E-04	-5.729292E-04	6.266125E-04
34	H11	-3.687089E-03	-7.376619E-04	6.463941E-04
35	H12	7.167595E-04	-2.611610E-03	-1.701288E-03

```
  36    H13    -2.454741E-03  -3.064387E-04  -3.360829E-03
 -----------   -------------  -------------  -------------
   total       -6.646360E-04   9.105446E-04  -7.935643E-05

  end of program der1b


  start of program geopt   6

  geometry optimization step  6
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3000057
   Cos(theta):   0.4865671

   Final level shift:  -2.0679667E-02

  energy change:          -6.0091E-05 .  (  5.0000E-05 )
  gradient maximum:        1.1941E-02 .  (  4.5000E-04 )
  gradient rms:            2.8233E-03 .  (  3.0000E-04 )
  step size:   0.30001  trust radius:   0.30000
  displacement maximum:    2.1374E-01 .  (  1.8000E-03 )
  displacement rms:        2.7161E-02 .  (  1.2000E-03 )
  predicted energy change:    -3.2067E-03    geom step:   3.0001E-
01    full step:   3.0001E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -3.3058E-02     y:    -1.3446E-03     z:     1.6301E-02

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.2021312988     1.8733743511    -2.2261144547
  C1       -1.1255300981     2.1104798051    -1.1782361265
  C2       -0.9102745047     2.6861819198     1.5058676311
  C3       -0.9124290353     1.0797978327    -0.2792332898
  C4       -1.2290724083     3.4233116265    -0.7560092991
  C5       -1.1177208234     3.7040865538     0.5923576427
  C6       -0.8114719283     1.3678030438     1.0820173903
  C7       -0.8087391363    -0.3562102400    -0.7524663245
  H3       -1.3878114642     4.2124612461    -1.4677803341
  H4       -1.1949163520     4.7159753806     0.9476472234
  H6       -0.8255493611     2.9305472908     2.5475908580
  C16       0.6022837697    -0.7535370452    -1.1899191655
  C8       -1.4336406315    -1.2526033232     0.3369945726
  N2       -0.5637103671     0.3334073534     2.0136689184
```

```
  C9       -0.7956297423     -0.9929152113      1.6879762432
  C10       0.0929368152      0.6482781831      3.2594973960
  O1       -0.5513110194     -1.8861532885      2.4529140673
  C23      -1.4259922500     -2.7395719352      0.0103902564
  C18       3.1485043573     -1.5525131582     -2.0444469350
  C19       0.7684953091     -1.4745126474     -2.3656648746
  C20       1.7376698281     -0.4324003000     -0.4518502747
  C21       2.9961970451     -0.8302669410     -0.8734338778
  C22       2.0288677439     -1.8729032033     -2.7902732400
  H2       -0.0926968795     -1.7320301703     -2.9597843583
  H5        1.6454268493      0.1352949207      0.4522972211
  H7        3.8591953660     -0.5660731327     -0.2873300396
  H8        2.1295850597     -2.4348298867     -3.7025797246
  H9        4.1281974348     -1.8578003269     -2.3708233964
  H10      -1.4477477314     -0.4525353223     -1.6280288760
  H19      -0.4164574236     -3.1435765529     -0.0080078994
  H20      -1.8716697775     -2.9041636420     -0.9654909832
  H21      -1.9855606783     -3.2892627045      0.7604786725
  H22      -2.4620713976     -0.9158141412      0.4385032208
  H11       1.0432823483      1.1389733622      3.0782337589
  H12       0.2588851987     -0.2845517033      3.7747974161
  H13      -0.5467107744      1.2846166991      3.8611557632

  nuclear repulsion energy.......  1417.469783671 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   6   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.293E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     87     84
82
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    183    195    183    183    188
176
```

```
  grid # 4      216    326    327    338    328    328    325
313

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     96     82
68
  grid # 2      118    118    109    100     90    107     91
78
  grid # 3      224    223    207    194    176    210    176
147
  grid # 4      224    223    206    341    310    391    294
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      122     80     97     95     96     97     96
112
  grid # 3      256    145    183    182    182    183    183
212
  grid # 4      448    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       70     73     73     73     66     70     72
70
  grid # 2      111    118    118    118    104    110    108
108
  grid # 3      209    222    223    224    203    217    216
217
  grid # 4      205    223    223    224    201    213    215
218

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     72     71     70   2865
  grid # 2      110    110    107    109   3722
  grid # 3      215    216    213    212   7177
  grid # 4      212    217    208    212   9916

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
  end of program rwr
```

```
  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  2  U  -783.01014976503           3.3E-04  1.0E-02
etot  2  Y  Y  6  M  -783.02926272450  1.9E-02  1.5E-04  4.0E-03
etot  3  N  Y  2  U  -783.03150688944  2.2E-03  4.2E-05  1.1E-03
etot  4  Y  Y  6  M  -783.03163588170  1.3E-04  1.9E-05  4.4E-04
etot  5  Y  Y  6  M  -783.03166035585  2.4E-05  5.9E-06  1.6E-04
etot  6  Y  Y  6  M  -783.03166072795  3.7E-07  3.1E-06  6.1E-05
etot  7  Y  N  6  M  -783.03166208404  1.4E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1417.46978367085
   (E)  Total one-electron terms..... -3879.48178181008
   (I)  Total two-electron terms.....  1678.98033605519
   (L)  Electronic energy............ -2200.50144575489  (E+I)
   (N)  Total energy.................  -783.03166208404  (A+L)

 SCFE: SCF energy: HF    -783.03166208404 hartrees   iterations:
7


 HOMO energy:    -0.30282
 LUMO energy:     0.12920

  Orbital energies:
  -20.52833  -15.59891  -11.34756  -11.28416  -11.25541  -11.25028
  -11.24282  -11.24110  -11.24097  -11.23778  -11.23734  -11.23401
  -11.23182  -11.23107  -11.23022  -11.22982  -11.22896  -11.22833
  -11.20996   -1.39587   -1.26968   -1.16613   -1.14985   -1.10741
   -1.03087   -1.01910   -1.01872   -1.01296   -0.96182   -0.93266
   -0.85779   -0.83758   -0.83380   -0.82208   -0.79653   -0.74064
   -0.71223   -0.69518   -0.67394   -0.66491   -0.64360   -0.63948
   -0.62761   -0.61484   -0.61282   -0.60999   -0.59844   -0.58336
   -0.57719   -0.55308   -0.54718   -0.53906   -0.53177   -0.51842
   -0.51574   -0.50780   -0.50089   -0.49848   -0.48554   -0.46816
   -0.46376   -0.42210   -0.41006   -0.34286   -0.33312   -0.32377
   -0.30282    0.12920    0.13420    0.14331    0.15250    0.20197
    0.22872    0.24015    0.24285    0.26249    0.28403

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
recomputing RwR matrix  14    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	5.082966E-05	4.147403E-04	2.390451E-04
2	C1	-2.524073E-04	-2.990812E-04	-3.991328E-04
3	C2	-5.991792E-05	2.355079E-03	2.679523E-03
4	C3	-2.392454E-04	-1.776242E-03	-1.464150E-03
5	C4	7.761207E-05	1.771058E-03	-1.012603E-03
6	C5	-2.711701E-04	7.174789E-04	6.043006E-04
7	C6	2.246728E-03	-4.134496E-04	1.492497E-04
8	C7	-1.798624E-03	2.172768E-03	-1.998846E-03
9	H3	-2.883140E-04	3.614995E-04	-4.275217E-04
10	H4	2.857580E-05	6.108377E-04	-4.015449E-04
11	H6	-4.417723E-04	8.065909E-05	-9.309747E-04
12	C16	-2.435824E-03	-1.149247E-03	5.727584E-04
13	C8	5.293563E-03	7.802561E-04	-9.210096E-04
14	N2	-2.519041E-03	-1.011425E-02	-1.662046E-02
15	C9	6.589599E-04	2.388519E-03	1.049986E-02
16	C10	-2.902421E-03	-4.428730E-03	6.574448E-03
17	O1	8.097711E-04	5.789901E-03	-2.604982E-03
18	C23	1.800907E-03	-3.873625E-03	1.666163E-03
19	C18	9.814273E-04	-6.533904E-04	-7.102130E-04
20	C19	1.862769E-03	-1.230075E-03	-1.876152E-03
21	C20	7.734895E-04	-8.375331E-04	-9.570674E-04
22	C21	-5.025218E-04	2.040601E-03	2.014484E-03
23	C22	-2.354383E-03	-7.166479E-04	-1.206419E-03
24	H2	4.437174E-04	1.868475E-04	3.441638E-04
25	H5	2.889637E-04	1.301402E-03	1.447727E-03
26	H7	-1.221190E-04	-2.383464E-04	2.095295E-04
27	H8	-5.534103E-06	2.916568E-04	-1.546134E-04
28	H9	-8.144565E-04	1.268940E-04	7.794458E-05
29	H10	1.883791E-03	-3.109749E-04	1.420457E-03
30	H19	-3.111543E-03	2.448036E-03	4.316898E-04
31	H20	-1.549001E-03	-7.695155E-04	3.875000E-04
32	H21	6.506813E-04	5.123084E-04	-2.844080E-03
33	H22	-2.342860E-03	4.099760E-05	-1.014200E-04
34	H11	-6.799325E-04	1.970137E-03	7.057778E-04
35	H12	6.858655E-04	2.579776E-03	1.639957E-03
36	H13	3.715259E-03	-8.931149E-04	2.937944E-03
total		-4.381795E-04	1.237225E-03	-2.867465E-05

```
  end of program der1b


  start of program geopt   7

  geometry optimization step  7
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3003895
   Cos(theta):   0.5186509

   Final level shift:  -8.0189587E-03

  energy change:          -6.3508E-04 .  (  5.0000E-05 )
  gradient maximum:        1.0660E-02 .  (  4.5000E-04 )
  gradient rms:            2.6430E-03 .  (  3.0000E-04 )
  step size:   0.30039  trust radius:   0.30000
  displacement maximum:    2.0077E-01 .  (  1.8000E-03 )
  displacement rms:        2.7196E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.6359E-03    geom step:   3.0039E-
01    full step:   3.0039E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     3.7293E-02     y:     3.5921E-03     z:    -1.8080E-02

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.2060637633     1.8844493579    -2.2172973329
  C1       -1.1162159815     2.1199748279    -1.1710457399
  C2       -0.8750562384     2.7005472519     1.5121309121
  C3       -0.8924559745     1.0856524139    -0.2759781118
  C4       -1.2172852275     3.4382213400    -0.7520106656
  C5       -1.0953405798     3.7182673439     0.5969574083
  C6       -0.7714985069     1.3761629880     1.0873596585
  C7       -0.8039986814    -0.3522858708    -0.7474083092
  H3       -1.3910485446     4.2238015270    -1.4647088856
  H4       -1.1760658928     4.7306083866     0.9492926346
  H6       -0.8001976785     2.9559921480     2.5483428251
  C16       0.5935061370    -0.7624401520    -1.2124886027
  C8       -1.3970841471    -1.2544925767     0.3579215937
  N2       -0.5302400873     0.3279037722     1.9981145627
  C9       -0.7517363528    -0.9839297206     1.7072076741
  C10      -0.1028905110     0.6226102755     3.3793777505
  O1       -0.4815390049    -1.8602482796     2.4710728185
  C23      -1.4069593418    -2.7445057154     0.0351543085
```

```
  C18       3.1164372369     -1.5703257625     -2.1047638215
  C19       0.7356291839     -1.5213338707     -2.3697245139
  C20       1.7450190202     -0.4027161135     -0.5167148879
  C21       2.9924975402     -0.8080217649     -0.9535065916
  C22       1.9823247445     -1.9214191571     -2.8168486051
  H2       -0.1393117586     -1.8030771280     -2.9301047588
  H5        1.6740918410      0.2123410873      0.3617379721
  H7        3.8670569792     -0.5263749433     -0.3950571846
  H8        2.0647440841     -2.5006478610     -3.7202071737
  H9        4.0865798413     -1.8814906020     -2.4452556976
  H10      -1.4542944640     -0.4550500198     -1.6047119739
  H19      -0.4146435807     -3.1003938955     -0.1239894694
  H20      -1.9948428207     -2.9377698958     -0.8553108722
  H21      -1.8383085739     -3.3040552640      0.8409012447
  H22      -2.4265389290     -0.9249000252      0.4740179438
  H11       0.8559945173      1.1410591180      3.3718041732
  H12      -0.0060463007     -0.3060975808      3.9061705905
  H13      -0.8139734314      1.2359193215      3.9289086681

  nuclear repulsion energy.......  1415.083079959 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   7   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.349E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     87     89     89     87     85
82
  grid # 2      116     96     96     98     97     97     93
90
  grid # 3      217    182    184    195    183    184    192
175
  grid # 4      216    326    329    337    328    328    326
312

  number of gridpoints:
```

```
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     94     81
70
  grid # 2      118    118    110    100     91    104     92
78
  grid # 3      224    223    208    194    176    213    175
147
  grid # 4      224    223    207    342    311    392    296
277

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     72     89     88     88     89     89
71
  grid # 2      122     80     97     95     96     97     96
112
  grid # 3      255    149    183    183    182    184    183
212
  grid # 4      447    280    327    326    327    327    327
212

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     68     71     71
70
  grid # 2      111    118    118    118    107    108    109
108
  grid # 3      211    223    223    224    202    215    217
217
  grid # 4      206    223    223    224    196    211    218
216

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     71     71   2863
  grid # 2      110    111    105    107   3719
  grid # 3      215    217    212    214   7193
  grid # 4      210    222    205    218   9919

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
```

	t e r	p d t	i i s	c u t	r i d	total energy	energy change	RMS density change	maximum DIIS error
etot	1	N	N	2	U	-783.00572045925		3.5E-04	1.5E-02
etot	2	Y	Y	6	M	-783.02816665484	2.2E-02	1.6E-04	4.2E-03
etot	3	N	Y	2	U	-783.03070115906	2.5E-03	4.5E-05	7.8E-04
etot	4	Y	Y	6	M	-783.03081424750	1.1E-04	2.0E-05	3.6E-04
etot	5	Y	Y	6	M	-783.03083834411	2.4E-05	5.6E-06	1.2E-04
etot	6	Y	Y	6	M	-783.03084494480	6.6E-06	2.6E-06	5.6E-05
etot	7	Y	N	6	M	-783.03084513822	1.9E-07	0.0E+00	0.0E+00

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1415.08307995899
   (E)  Total one-electron terms..... -3874.74976358586
   (I)  Total two-electron terms.....  1676.63583848865
   (L)  Electronic energy..... -2198.11392509721  (E+I)
   (N)  Total energy.................  -783.03084513822  (A+L)

 SCFE: SCF energy: HF    -783.03084513822 hartrees   iterations:
7


 HOMO energy:    -0.30150
 LUMO energy:     0.12931

  Orbital energies:
  -20.52623  -15.60196  -11.34425  -11.28806  -11.25773  -11.24924
  -11.24162  -11.24070  -11.23969  -11.23864  -11.23801  -11.23524
  -11.23042  -11.23002  -11.22950  -11.22874  -11.22771  -11.22676
  -11.20467   -1.40154   -1.26972   -1.16455   -1.14832   -1.10546
   -1.03009   -1.01848   -1.01701   -1.01269   -0.96167   -0.93376
   -0.85901   -0.84075   -0.83279   -0.82104   -0.79613   -0.74203
   -0.71118   -0.69452   -0.67376   -0.66400   -0.64413   -0.63721
   -0.62740   -0.61423   -0.61191   -0.60811   -0.59521   -0.58350
   -0.57605   -0.55229   -0.54975   -0.54154   -0.53339   -0.51841
   -0.51440   -0.50726   -0.50082   -0.49703   -0.48429   -0.46907
   -0.46212   -0.42392   -0.41099   -0.34214   -0.33278   -0.32190
   -0.30150    0.12931    0.13453    0.14496    0.15196    0.20661
    0.23155    0.24129    0.24929    0.26183    0.28792

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr
```

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	-1.345234E-04	-1.287784E-04	-4.775301E-04
2	C1	2.789039E-04	9.842413E-04	7.887341E-04
3	C2	-4.454131E-04	-1.500603E-03	-1.869518E-03
4	C3	1.336679E-05	2.075056E-03	4.323622E-04
5	C4	2.872991E-04	-2.631794E-03	7.206142E-04
6	C5	2.363437E-04	-1.740103E-03	-1.125056E-03
7	C6	-2.338580E-03	1.869163E-03	-3.262312E-03
8	C7	2.514015E-03	-1.379252E-03	1.611937E-03
9	H3	9.566931E-05	1.625675E-04	-7.817488E-05
10	H4	5.338242E-05	5.588807E-04	4.099372E-04
11	H6	1.083146E-03	-1.064019E-03	2.175652E-03
12	C16	3.847128E-04	1.349993E-03	3.891506E-04
13	C8	-1.239438E-03	-1.185052E-03	-7.314713E-04
14	N2	2.132938E-03	1.213271E-02	2.634140E-02
15	C9	-2.391581E-03	-2.574927E-03	-1.649513E-02
16	C10	3.852591E-03	7.134513E-03	-5.669553E-03
17	O1	-6.082847E-05	-8.808798E-03	6.847289E-03
18	C23	-6.031663E-03	6.963073E-03	-2.644129E-03
19	C18	4.804597E-04	-4.972846E-05	-5.994728E-05
20	C19	-2.895783E-03	9.203431E-04	7.784932E-04
21	C20	-2.011694E-03	1.323757E-03	5.652296E-04
22	C21	7.449429E-04	-1.349202E-03	-1.237316E-03
23	C22	1.919302E-03	-1.397776E-04	-1.477727E-04
24	H2	-4.006863E-04	1.259212E-04	-1.176327E-04
25	H5	-1.628250E-04	-8.441868E-04	1.083419E-04
26	H7	6.662561E-04	3.013372E-04	-8.538325E-05
27	H8	2.557648E-04	-2.100563E-04	3.790917E-04
28	H9	1.210621E-03	-2.590803E-04	-4.148695E-04
29	H10	-2.076596E-03	-6.321162E-05	-2.071245E-03
30	H19	1.066426E-02	-5.735758E-03	-1.786585E-03
31	H20	2.561933E-04	1.331208E-03	-2.289656E-03
32	H21	-2.611967E-03	-2.890473E-03	6.415145E-03
33	H22	-2.481258E-03	1.099190E-03	9.964031E-04
34	H11	-3.261198E-03	-1.761278E-03	-4.250366E-04
35	H12	2.359964E-03	-2.376032E-03	-1.358300E-03
36	H13	-1.865198E-03	-8.414605E-04	-6.861972E-03
total		-9.190946E-04	7.983831E-04	-2.488093E-04

end of program der1b

start of program geopt 8

geometry optimization step 8

```
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3000105
   Cos(theta):   0.6019445

   Final level shift:  -3.4583305E-02

  energy change:           8.1695E-04 .  (  5.0000E-05 )
  gradient maximum:        1.7826E-02 .  (  4.5000E-04 )
  gradient rms:            3.8954E-03 .  (  3.0000E-04 )
  step size:   0.30001  trust radius:   0.30000
  displacement maximum:    1.5218E-01 .  (  1.8000E-03 )
  displacement rms:        2.7162E-02 .  (  1.2000E-03 )
  predicted energy change:    -5.4413E-03    geom step:   3.0001E-
01    full step:   3.0001E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -3.4466E-02     y:    -5.9815E-03     z:     1.7508E-02

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.2046544007     1.8783275428    -2.2228604213
  C1       -1.1243695996     2.1127377444    -1.1747909746
  C2       -0.8964629456     2.6844650961     1.5101826733
  C3       -0.9142935064     1.0798661829    -0.2774911322
  C4       -1.2201716188     3.4250106923    -0.7518060154
  C5       -1.1010717672     3.7037057576     0.5969715524
  C6       -0.8090470103     1.3663334697     1.0845569784
  C7       -0.8099732815    -0.3560479331    -0.7529817026
  H3       -1.3793438780     4.2157761767    -1.4624649722
  H4       -1.1701965204     4.7171074317     0.9513827764
  H6       -0.8058809644     2.9242078411     2.5522679888
  C16       0.5982578365    -0.7525453092    -1.1967210184
  C8       -1.4304494145    -1.2560574070     0.3369748268
  N2       -0.5503505571     0.3300890385     2.0187476874
  C9       -0.7917989037    -0.9974430376     1.6910903953
  C10       0.0658971114     0.6636049639     3.2785163802
  O1       -0.5615427370    -1.8898753909     2.4619783932
  C23      -1.4240370128    -2.7482515775     0.0129995912
  C18       3.1472190383    -1.5512187283    -2.0578023781
  C19       0.7625109496    -1.4777047321    -2.3712785576
  C20       1.7358677836    -0.4279934029    -0.4650571640
  C21       2.9952612075    -0.8250544434    -0.8900522524
  C22       2.0242078050    -1.8760779298    -2.7991041086
  H2       -0.1007956422    -1.7347833321    -2.9631965287
```

```
  H5        1.6497417316      0.1399239247      0.4399363337
  H7        3.8604520927     -0.5581662244     -0.3078243962
  H8        2.1237606030     -2.4388267225     -3.7090496169
  H9        4.1271700966     -1.8547407860     -2.3849372462
  H10      -1.4505018669     -0.4546740579     -1.6268754035
  H19      -0.4086254961     -3.1617404324     -0.0113461399
  H20      -1.8708786231     -2.9072278620     -0.9639818605
  H21      -1.9910798153     -3.2980126072      0.7652698506
  H22      -2.4651524546     -0.9182164199      0.4429340545
  H11       0.9785511247      1.2228720066      3.1067170873
  H12       0.3051799025     -0.2577449189      3.7832726892
  H13      -0.6265580817      1.2442585545      3.8716199658

  nuclear repulsion energy.......  1416.059050702 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   8   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.308E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     87     84
81
  grid # 2      116     96     96     98     97     97     94
91
  grid # 3      216    182    184    195    184    184    187
176
  grid # 4      216    326    327    338    328    328    324
312

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     97     82
68
  grid # 2      118    118    109    100     90    105     91
78
```

```
  grid # 3      224    223    207    196    173    213    176
146
  grid # 4      224    223    206    341    312    391    295
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     87     89     89
71
  grid # 2      123     81     97     95     96     97     96
112
  grid # 3      256    147    183    182    182    183    183
212
  grid # 4      450    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       70     73     73     73     66     70     72
70
  grid # 2      111    118    118    118    106    110    108
109
  grid # 3      210    222    223    223    203    217    216
217
  grid # 4      205    223    224    224    201    218    215
221

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     70   2861
  grid # 2      111    108    108    108   3724
  grid # 3      215    215    213    212   7180
  grid # 4      213    212    210    210   9922

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d    total energy      change  change    error

etot   1  N  N  2  U  -783.00842820834           3.3E-04  1.1E-02
etot   2  Y  Y  6  M  -783.02900799999  2.1E-02  1.5E-04  3.2E-03
```

```
etot   3  N  Y  2  U  -783.03123948088  2.2E-03  4.1E-05  7.4E-04
etot   4  Y  Y  6  M  -783.03136999434  1.3E-04  1.9E-05  2.9E-04
etot   5  Y  Y  6  M  -783.03138474704  1.5E-05  5.1E-06  1.1E-04
etot   6  Y  Y  6  M  -783.03138431173 -4.4E-07  2.3E-06  4.9E-05
etot   7  Y  N  6  M  -783.03138353949 -7.7E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1416.05905070195
   (E)  Total one-electron terms..... -3876.68109013092
   (I)  Total two-electron terms.....  1677.59065588948
   (L)  Electronic energy............. -2199.09043424144  (E+I)
   (N)  Total energy.................  -783.03138353949  (A+L)

 SCFE: SCF energy: HF    -783.03138353949 hartrees   iterations:
7


 HOMO energy:    -0.30265
 LUMO energy:     0.12931

  Orbital energies:
  -20.52812  -15.59889  -11.34801  -11.28462  -11.25559  -11.25054
  -11.24470  -11.24133  -11.24111  -11.23810  -11.23742  -11.23403
  -11.23203  -11.23096  -11.23057  -11.22984  -11.22896  -11.22818
  -11.21238   -1.39469   -1.26819   -1.16578   -1.14959   -1.10662
   -1.02988   -1.01907   -1.01861   -1.01219   -0.96231   -0.93196
   -0.85694   -0.83668   -0.83365   -0.82194   -0.79616   -0.73977
   -0.71129   -0.69513   -0.67323   -0.66430   -0.64348   -0.63932
   -0.62745   -0.61467   -0.61323   -0.60922   -0.59878   -0.58280
   -0.57710   -0.55327   -0.54673   -0.53941   -0.53154   -0.51776
   -0.51547   -0.50711   -0.50066   -0.49824   -0.48522   -0.46812
   -0.46355   -0.42096   -0.41046   -0.34293   -0.33254   -0.32392
   -0.30265    0.12931    0.13426    0.14323    0.15242    0.20170
    0.22876    0.24024    0.24366    0.26202    0.28422

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x              y              z
```

1	H1	6.754269E-05	1.484976E-04	1.625033E-04
2	C1	-4.297930E-04	-1.214185E-03	-6.459060E-04
3	C2	-6.436097E-04	2.488579E-03	2.043006E-03
4	C3	5.384116E-05	-2.382377E-03	-9.098488E-04
5	C4	2.949671E-05	2.639026E-03	6.296979E-05
6	C5	-6.020940E-04	1.542792E-03	3.559638E-04
7	C6	4.443763E-03	-3.025602E-03	2.277508E-03
8	C7	-2.623202E-03	1.241934E-03	-2.062676E-03
9	H3	-7.535924E-05	1.106751E-04	-1.083848E-04
10	H4	3.564563E-05	1.608811E-04	-3.196634E-04
11	H6	-4.600136E-04	7.003288E-04	-1.065761E-03
12	C16	-1.329877E-03	-1.575709E-03	2.918836E-04
13	C8	3.231682E-03	5.320824E-04	1.130432E-03
14	N2	-5.739442E-03	-1.037996E-02	-2.368114E-02
15	C9	6.253407E-04	3.849334E-03	1.336909E-02
16	C10	-3.214380E-06	-5.337077E-03	3.019446E-03
17	O1	9.943650E-04	6.770482E-03	-3.665438E-03
18	C23	4.346059E-03	-5.029903E-03	2.386789E-03
19	C18	-6.780674E-04	-7.293570E-04	-1.277954E-03
20	C19	3.303251E-03	-1.180330E-03	-2.227864E-03
21	C20	2.902467E-03	-1.012561E-03	-4.530768E-04
22	C21	-1.043674E-03	2.360615E-03	2.716621E-03
23	C22	-3.415880E-03	6.355409E-04	6.712632E-04
24	H2	7.986165E-04	-6.321815E-05	4.191238E-04
25	H5	-1.373954E-04	1.328309E-03	1.140928E-03
26	H7	-4.933481E-04	-9.530353E-05	3.111275E-04
27	H8	-1.301729E-04	-4.145972E-04	-1.215579E-03
28	H9	-9.299230E-04	1.085227E-05	-1.021287E-04
29	H10	1.474780E-03	5.719194E-05	1.336150E-03
30	H19	-8.745452E-03	5.231834E-03	1.271904E-03
31	H20	-1.490535E-03	-1.184151E-03	8.172839E-04
32	H21	3.097514E-03	2.459154E-03	-5.330651E-03
33	H22	1.894296E-03	-1.603354E-03	-5.055083E-04
34	H11	-6.101446E-04	2.528858E-03	1.660908E-03
35	H12	-1.149873E-03	1.027478E-03	1.774567E-03
36	H13	2.901508E-03	5.304608E-04	6.026358E-03
total		-5.309006E-04	1.127220E-03	-3.257527E-04

```
 end of program der1b


 start of program geopt   9

 geometry optimization step  9
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
```

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3000251
   Cos(theta):   0.5877516

   Final level shift:  -1.6600358E-02

  energy change:          -5.3840E-04 .  (  5.0000E-05 )
  gradient maximum:        1.6089E-02 .  (  4.5000E-04 )
  gradient rms:            3.5564E-03 .  (  3.0000E-04 )
  step size:   0.30002  trust radius:   0.30000
  displacement maximum:    1.6821E-01 .  (  1.8000E-03 )
  displacement rms:        2.7163E-02 .  (  1.2000E-03 )
  predicted energy change:    -4.2106E-03    geom step:   3.0002E-
01    full step:   3.0002E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     3.3972E-02     y:     7.2210E-03     z:    -1.7067E-02

  new geometry:
                                angstroms
  atom            x                 y                 z
  H1       -1.1959850689     1.8795569850     -2.2163864898
  C1       -1.1058669005     2.1165747112     -1.1701107483
  C2       -0.8629608188     2.7026453295      1.5109337136
  C3       -0.8880331061     1.0823927154     -0.2739293177
  C4       -1.1996358749     3.4370094468     -0.7526780514
  C5       -1.0771853730     3.7204439472      0.5945444137
  C6       -0.7666563274     1.3761729362      1.0877031786
  C7       -0.8040118379    -0.3559018865     -0.7432415345
  H3       -1.3669527525     4.2218421616     -1.4673583848
  H4       -1.1506622511     4.7339120586      0.9452669176
  H6       -0.7842105134     2.9578197917      2.5478949008
  C16       0.5916610455    -0.7644552035     -1.2164015847
  C8       -1.3857221944    -1.2605938980      0.3648262832
  N2       -0.5375433964     0.3345655612      2.0010423720
  C9       -0.7550822887    -0.9790135830      1.7173290553
  C10      -0.1397548261     0.6385257597      3.3883422090
  O1       -0.4959221837    -1.8504114624      2.4923108672
  C23      -1.3743288698    -2.7469563729      0.0408887661
  C18       3.1027208973    -1.5786553471     -2.1238429505
  C19       0.7249206683    -1.5102659123     -2.3823009527
  C20       1.7472145942    -0.4174307585     -0.5180046152
  C21       2.9894349876    -0.8270758521     -0.9623860172
  C22       1.9655602266    -1.9125728494     -2.8376989177
  H2       -0.1532918518    -1.7823533997     -2.9410759245
  H5        1.6783588193     0.1904690514      0.3667184589
  H7        3.8674203198    -0.5581005888     -0.4029168141
  H8        2.0415264326    -2.4832325233     -3.7493477133
  H9        4.0690900406    -1.8941325491     -2.4721630135
  H10      -1.4608766959    -0.4583672943     -1.5967324249
  H19      -0.3811010265    -3.0803581605     -0.1344219107
```

```
  H20      -1.9752202314     -2.9546306528     -0.8382877628
  H21      -1.7752467624     -3.3127663558      0.8538292519
  H22      -2.4169242325     -0.9495434889      0.4793171546
  H11       0.7705770407      1.2340780346      3.4044492063
  H12       0.0255953980     -0.2974783874      3.8893732053
  H13      -0.9012479159      1.1766093674      3.9554405678

  nuclear repulsion energy.......  1415.332104438 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   9   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.348E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     87     89     89     87     86
82
  grid # 2      116     96     96     98     97     97     94
90
  grid # 3      217    184    184    195    183    183    192
175
  grid # 4      216    326    330    337    328    328    329
312

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     96     81
72
  grid # 2      118    118    111    100     91    104     92
79
  grid # 3      224    223    208    193    177    213    176
145
  grid # 4      224    223    208    340    310    391    295
275

  number of gridpoints:
```

```
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     72     89     88     88     89     89
71
  grid # 2      122     80     97     95     96     97     96
112
  grid # 3      255    149    183    183    183    184    183
212
  grid # 4      447    283    327    325    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     70     71
69
  grid # 2      111    118    118    118    106    108    109
108
  grid # 3      211    223    223    224    203    215    217
217
  grid # 4      207    223    223    224    197    210    218
213

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     71     71   2863
  grid # 2      110    108    105    109   3720
  grid # 3      216    215    211    215   7194
  grid # 4      207    218    204    222   9912

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  2  U  -783.00503434625           3.6E-04  1.4E-02
etot  2  Y  Y  6  M  -783.02804818392  2.3E-02  1.6E-04  4.1E-03
etot  3  N  Y  2  U  -783.03054845712  2.5E-03  4.4E-05  6.3E-04
etot  4  Y  Y  6  M  -783.03065869193  1.1E-04  2.0E-05  2.5E-04
etot  5  Y  Y  6  M  -783.03068037353  2.2E-05  5.4E-06  1.0E-04
etot  6  Y  Y  6  M  -783.03068475585  4.4E-06  2.3E-06  4.1E-05
etot  7  Y  N  6  M  -783.03068421268 -5.4E-07  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1415.33210443810
   (E)  Total one-electron terms..... -3875.22658025810
   (I)  Total two-electron terms.....  1676.86379160732
   (L)  Electronic energy..... -2198.36278865078  (E+I)
   (N)  Total energy.............  -783.03068421268  (A+L)

 SCFE: SCF energy: HF    -783.03068421268 hartrees   iterations:
7


 HOMO energy:    -0.30095
 LUMO energy:     0.12923

  Orbital energies:
 -20.52683  -15.60247  -11.34501  -11.28753  -11.25779  -11.24922
 -11.24114  -11.24007  -11.23975  -11.23836  -11.23791  -11.23492
 -11.23044  -11.22991  -11.22958  -11.22848  -11.22795  -11.22718
 -11.20347   -1.40175   -1.27145   -1.16484   -1.14827   -1.10611
  -1.03090   -1.01804   -1.01710   -1.01326   -0.96193   -0.93408
  -0.85994   -0.84133   -0.83270   -0.82117   -0.79628   -0.74249
  -0.71167   -0.69456   -0.67397   -0.66427   -0.64436   -0.63721
  -0.62761   -0.61424   -0.61223   -0.60833   -0.59572   -0.58410
  -0.57588   -0.55222   -0.54984   -0.54175   -0.53307   -0.51885
  -0.51433   -0.50761   -0.50097   -0.49706   -0.48437   -0.46924
  -0.46216   -0.42457   -0.41160   -0.34216   -0.33338   -0.32160
  -0.30095    0.12923    0.13450    0.14503    0.15217    0.20620
   0.23167    0.24163    0.25052    0.26131    0.28968

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  14    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1     H1     -1.373718E-04   1.030495E-04  -2.484581E-04
   2     C1      3.244042E-04   1.883872E-03   6.820277E-04
   3     C2     -2.992705E-04  -1.923170E-03  -1.487067E-03
```

4	C3	-2.694873E-04	2.639274E-03	1.036148E-04
5	C4	2.112426E-04	-3.332747E-03	-7.317086E-04
6	C5	6.139853E-04	-2.184378E-03	-2.695905E-04
7	C6	-3.701372E-03	4.836635E-03	-4.408113E-03
8	C7	2.911239E-03	-6.881624E-04	1.423238E-03
9	H3	-4.052756E-05	2.635351E-04	-2.743812E-04
10	H4	-1.610996E-05	5.600404E-04	2.851475E-04
11	H6	6.420110E-04	-1.214374E-03	1.545260E-03
12	C16	1.509192E-04	1.891438E-03	7.480516E-04
13	C8	-8.239532E-05	-5.963336E-04	-1.682294E-03
14	N2	3.612162E-03	1.138460E-02	2.910671E-02
15	C9	-1.239325E-03	-4.621613E-03	-1.542498E-02
16	C10	1.418085E-03	3.728804E-03	-2.223565E-03
17	O1	-6.848788E-04	-7.252304E-03	5.733728E-03
18	C23	-7.719663E-03	6.511866E-03	-3.057802E-03
19	C18	1.780575E-03	5.493529E-04	6.351478E-04
20	C19	-4.179016E-03	1.313615E-03	1.524875E-03
21	C20	-4.099859E-03	1.397866E-03	2.904105E-04
22	C21	1.169174E-03	-2.014899E-03	-2.264286E-03
23	C22	3.487780E-03	-1.519380E-03	-1.769026E-03
24	H2	-8.613886E-04	1.910902E-04	-3.446411E-04
25	H5	2.466087E-04	-1.334368E-03	-3.339408E-04
26	H7	7.654884E-04	1.613000E-04	-3.385733E-04
27	H8	2.954715E-04	5.523869E-04	1.599179E-03
28	H9	1.116291E-03	-7.224874E-05	-8.595172E-05
29	H10	-1.524094E-03	-2.803361E-04	-1.551203E-03
30	H19	1.349237E-02	-6.842007E-03	-2.804427E-03
31	H20	5.534243E-04	1.699099E-03	-2.006370E-03
32	H21	-3.697573E-03	-4.279422E-03	8.034846E-03
33	H22	-5.182788E-03	2.421745E-03	1.094322E-03
34	H11	-1.873151E-03	-2.110829E-03	-1.772787E-03
35	H12	3.083038E-03	1.088651E-04	-1.045174E-03
36	H13	-1.106393E-03	-1.209954E-03	-8.539752E-03
total		-8.403957E-04	7.219079E-04	1.424752E-04

```
  end of program der1b


  start of program geopt  10

  geometry optimization step 10

 the energy is increasing and lowest energy was more than two
iters back                                    .

  [ turning on trust-radius adjustment ]
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  ** restarting optimization from step    7 **
```

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.1503519
   Cos(theta):   0.7290870

   Final level shift:  -4.0272366E-02

  energy change:           6.9933E-04 .  (  5.0000E-05 )
  gradient maximum:        1.0660E-02 .  (  4.5000E-04 )
  gradient rms:            2.6430E-03 .  (  3.0000E-04 )
  step size:   0.15035  trust radius:   0.15000
  displacement maximum:    9.6272E-02 .  (  1.8000E-03 )
  displacement rms:        1.3612E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.0552E-03    geom step:   1.5035E-
01    full step:   1.5035E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -3.4694E-17     y:     1.1796E-16     z:     1.1102E-16

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1965263362     1.8855691282    -2.2298047204
  C1       -1.1115434868     2.1196906157    -1.1825132679
  C2       -0.8848870881     2.6957352422     1.5031621409
  C3       -0.8842842539     1.0857492053    -0.2883100009
  C4       -1.2217745024     3.4353343717    -0.7595924593
  C5       -1.1079389037     3.7140467557     0.5902985093
  C6       -0.7704703680     1.3745219842     1.0745248479
  C7       -0.7906360499    -0.3520753742    -0.7584719661
  H3       -1.3954257839     4.2227433276    -1.4708656554
  H4       -1.1963637147     4.7254932682     0.9450632404
  H6       -0.8085686509     2.9436459962     2.5426488187
  C16       0.6112720270    -0.7616143622    -1.2095637340
  C8       -1.3978793591    -1.2500125901     0.3429212699
  N2       -0.5305927771     0.3310127766     1.9943046677
  C9       -0.7564671663    -0.9832207873     1.6935306299
  C10       0.0035891273     0.6401001546     3.3222429426
  O1       -0.4916217429    -1.8634405147     2.4569779987
  C23      -1.4089741134    -2.7395226939     0.0182194197
  C18       3.1416646165    -1.5707635243    -2.0803820407
  C19       0.7648259694    -1.4935607298    -2.3821695916
  C20       1.7543025934    -0.4309040148    -0.4857614877
  C21       3.0053824643    -0.8347404848    -0.9138283550
  C22       2.0155526546    -1.8966509362    -2.8166195489
  H2       -0.1035170440    -1.7523704637    -2.9647847202
  H5        1.6736777196     0.1577096474     0.4096372705
  H7        3.8741159092    -0.5707001654    -0.3374777491
  H8        2.1069833442    -2.4629255042    -3.7275007193
  H9        4.1153489493    -1.8827665741    -2.4122475273
```

```
  H10      -1.4351992504     -0.4535906415     -1.6228220717
  H19      -0.4081118344     -3.1226284864     -0.0613784478
  H20      -1.9276262059     -2.9162422832     -0.9187542167
  H21      -1.9140437425     -3.2917283475      0.7927312454
  H22      -2.4272183048     -0.9140056574      0.4515085466
  H11       0.9425523571      1.1839804530      3.2351894634
  H12       0.1689117525     -0.2865131295      3.8396965754
  H13      -0.6878268681      1.2350095685      3.9151050647

  nuclear repulsion energy.......  1415.888913871 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  10   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.341E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     87     89     89     87     83
82
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    195    183    184    191
176
  grid # 4      216    326    329    338    328    328    325
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     95     82
70
  grid # 2      118    118    110    100     91    104     92
78
  grid # 3      224    223    208    194    176    212    176
149
  grid # 4      224    223    207    342    311    391    291
279
```

```
  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      122     80     97     95     96     97     96
112
  grid # 3      256    147    183    183    182    184    183
212
  grid # 4      449    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       70     73     73     73     66     70     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      210    223    223    224    203    217    218
216
  grid # 4      205    223    223    224    197    212    217
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2859
  grid # 2      110    110    105    107   3721
  grid # 3      214    216    212    213   7193
  grid # 4      211    221    208    217   9924

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                              RMS    maximum
      t  p  i  c  r                                  energy  density   DIIS
      e  d  i  u  i                 total energy     change  change    error

etot  1  N  N  2  U  -783.02284735130              2.2E-04  9.4E-03
etot  2  Y  Y  6  M  -783.03152276544  8.7E-03  9.5E-05  2.6E-03
etot  3  N  Y  2  U  -783.03246863783  9.5E-04  2.6E-05  4.4E-04
etot  4  Y  Y  6  M  -783.03251086369  4.2E-05  1.0E-05  1.2E-04
etot  5  Y  Y  6  M  -783.03251580557  4.9E-06  2.9E-06  4.3E-05
etot  6  Y  N  6  M  -783.03251488581 -9.2E-07  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1415.88891387138
   (E)  Total one-electron terms..... -3876.35266144715
   (I)  Total two-electron terms.....  1677.43123268996
   (L)  Electronic energy..... -2198.92142875719  (E+I)
   (N)  Total energy.............  -783.03251488581  (A+L)

 SCFE: SCF energy: HF    -783.03251488581 hartrees   iterations:
6


 HOMO energy:    -0.30209
 LUMO energy:     0.12905

  Orbital energies:
 -20.52625  -15.60077  -11.34476  -11.28667  -11.25734  -11.24954
 -11.24156  -11.24147  -11.24018  -11.23863  -11.23807  -11.23508
 -11.23092  -11.23034  -11.22996  -11.22927  -11.22815  -11.22727
 -11.20700   -1.40001   -1.26972   -1.16499   -1.14871   -1.10591
  -1.03006   -1.01834   -1.01751   -1.01306   -0.96223   -0.93312
  -0.85836   -0.83982   -0.83303   -0.82137   -0.79629   -0.74142
  -0.71145   -0.69473   -0.67357   -0.66416   -0.64422   -0.63790
  -0.62738   -0.61437   -0.61160   -0.60883   -0.59627   -0.58369
  -0.57616   -0.55245   -0.54904   -0.54029   -0.53261   -0.51907
  -0.51498   -0.50736   -0.50074   -0.49783   -0.48461   -0.46871
  -0.46264   -0.42257   -0.41074   -0.34226   -0.33322   -0.32233
  -0.30209    0.12905    0.13415    0.14479    0.15224    0.20564
   0.23009    0.24096    0.24653    0.26195    0.28652

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr



  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1     -7.415435E-05   3.037119E-05  -2.236462E-04
   2    C1      2.934148E-04   9.479030E-04   5.894910E-04
   3    C2      2.683531E-04  -8.312424E-04  -1.017328E-03
```

```
 4    C3     -1.487681E-04   1.086158E-03   2.431753E-04
 5    C4      1.244034E-04  -1.603484E-03   1.121363E-04
 6    C5      3.763030E-04  -9.202544E-04  -5.171245E-04
 7    C6     -2.312182E-03   2.080362E-03  -1.112723E-03
 8    C7      1.174684E-03  -6.107119E-04   8.607345E-04
 9    H3      5.504253E-06  -9.140865E-05   4.033519E-05
10    H4      9.625167E-05   2.110069E-04   8.111222E-05
11    H6      3.129851E-04  -6.200578E-04   8.663554E-04
12    C16    -3.689890E-04   6.991416E-04   3.321559E-04
13    C8     -6.907380E-04  -1.510829E-04  -1.315335E-03
14    N2      3.561948E-03   7.594461E-03   1.131450E-02
15    C9     -1.189842E-03  -5.168063E-04  -8.515025E-03
16    C10     6.571713E-05   3.378263E-03  -1.150722E-03
17    O1      1.692355E-04  -6.273977E-03   5.179403E-03
18    C23    -2.319084E-03   3.260714E-03  -1.060312E-03
19    C18     5.699694E-04  -4.172793E-04  -2.911476E-04
20    C19    -2.493668E-03   5.706252E-04   4.862085E-04
21    C20    -1.898528E-03   1.128855E-03   4.770101E-04
22    C21     8.983130E-04  -6.948315E-04  -8.897197E-04
23    C22     1.778971E-03  -5.653975E-04  -3.899443E-04
24    H2      8.666562E-05   9.790290E-05   3.166642E-04
25    H5     -6.217467E-05  -4.698643E-04  -7.563567E-05
26    H7      4.488473E-04   8.066850E-05   4.800551E-05
27    H8      2.436248E-04   2.238760E-04   2.514228E-04
28    H9      6.231766E-04  -1.297313E-04  -2.963009E-04
29    H10    -9.038365E-04  -1.645274E-04  -1.022606E-03
30    H19     4.860259E-03  -2.781635E-03  -9.380783E-04
31    H20     3.986399E-04   5.906100E-04  -9.201650E-04
32    H21    -1.619973E-03  -1.315983E-03   2.955558E-03
33    H22    -1.732369E-03   5.198598E-04   5.420193E-04
34    H11    -2.633893E-03  -1.009749E-03  -3.686263E-04
35    H12     1.591662E-03  -1.183732E-03  -8.915990E-04
36    H13    -1.770045E-04  -1.172144E-03  -3.863008E-03
-----------   -------------  -------------  -------------
   total      -6.762774E-04   9.768783E-04  -1.627534E-04

 end of program der1b


 start of program geopt  11

 geometry optimization step 11
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0756353
  Cos(theta):   0.7626382
```

```
 Final level shift:  -8.3692244E-02

  energy change:          -8.5280E-04 .  (  5.0000E-05 )
  gradient maximum:        8.3698E-03 .  (  4.5000E-04 )
  gradient rms:            1.9294E-03 .  (  3.0000E-04 )
  step size:   0.07564  trust radius:   0.07500
  displacement maximum:    3.8408E-02 .  (  1.8000E-03 )
  displacement rms:        6.8477E-03 .  (  1.2000E-03 )
  predicted energy change:    -8.5404E-04    geom step:   7.5635E-
02    full step:   7.5635E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -7.5400E-03     y:    -1.6054E-03     z:     4.7227E-03

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -1.1925017276      1.8826081976     -2.2294416364
  C1       -1.1093829937      2.1173065617     -1.1819863078
  C2       -0.8852742304      2.6923260066      1.5030138270
  C3       -0.8900752082      1.0847098278     -0.2859055520
  C4       -1.2134745855      3.4309942606     -0.7598270701
  C5       -1.0994482320      3.7102571935      0.5892878767
  C6       -0.7794293310      1.3735884709      1.0762067079
  C7       -0.7934749209     -0.3532481356     -0.7575339651
  H3       -1.3804401178      4.2190959355     -1.4712499741
  H4       -1.1807368421      4.7225208510      0.9430883104
  H6       -0.8057456291      2.9366937169      2.5436965141
  C16       0.6106626470     -0.7586894262     -1.2063692779
  C8       -1.4077528813     -1.2501470418      0.3393248581
  N2       -0.5310790914      0.3330251795      2.0010752581
  C9       -0.7657099301     -0.9887147463      1.6911655999
  C10       0.0287723219      0.6502908161      3.3045254975
  O1       -0.5196715210     -1.8762777587      2.4594219877
  C23      -1.4106576091     -2.7409884857      0.0155044091
  C18       3.1501850169     -1.5636479631     -2.0775989773
  C19       0.7679768137     -1.4870460757     -2.3800598934
  C20       1.7526321050     -0.4315560861     -0.4812277891
  C21       3.0076161366     -0.8327053658     -0.9100094586
  C22       2.0242182949     -1.8882973534     -2.8139109308
  H2       -0.0985127616     -1.7460513447     -2.9650305728
  H5        1.6714230491      0.1480722095      0.4179444553
  H7        3.8754911865     -0.5672003216     -0.3315442456
  H8        2.1181242522     -2.4505839486     -3.7254127581
  H9        4.1263396729     -1.8712480862     -2.4090735391
  H10      -1.4360386194     -0.4534641485     -1.6263503116
  H19      -0.4033713645     -3.1377417631     -0.0386607895
  H20      -1.8967539122     -2.9117198172     -0.9397041310
  H21      -1.9430909938     -3.2909599198      0.7817172649
  H22      -2.4392500465     -0.9127869448      0.4472138934
  H11       0.9470880126      1.2166799198      3.1860172758
```

```
  H12       0.2404992749     -0.2765714672      3.8083321975
  H13      -0.6748350429      1.2224247433      3.8983069680

  nuclear repulsion energy.......  1415.778347722 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  11   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.312E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     87     83
81
  grid # 2      116     96     96     98     97     97     94
90
  grid # 3      216    182    183    194    183    184    189
176
  grid # 4      216    326    328    338    328    328    325
312

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     95     82
69
  grid # 2      118    118    110    100     90    105     92
79
  grid # 3      224    223    207    194    174    211    176
145
  grid # 4      224    223    207    342    311    390    293
277

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
```

```
  grid # 2      122     81     97     95     96     97     96
112
  grid # 3      256    148    183    182    182    183    183
212
  grid # 4      448    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       70     73     73     73     66     70     71
70
  grid # 2      111    118    118    118    106    109    110
108
  grid # 3      210    222    223    224    201    218    216
217
  grid # 4      205    223    223    224    196    215    217
216

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     71     71   2861
  grid # 2      110    110    107    108   3725
  grid # 3      215    216    214    213   7179
  grid # 4      213    215    208    212   9915

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  2  U  -783.03169748385           8.7E-05  2.2E-03
etot   2  Y  Y  6  M  -783.03283974474  1.1E-03  3.6E-05  6.8E-04
etot   3  Y  Y  6  M  -783.03295741274  1.2E-04  1.0E-05  1.5E-04
etot   4  Y  Y  6  M  -783.03296983025  1.2E-05  4.6E-06  5.6E-05
etot   5  Y  N  6  M  -783.03297148991  1.7E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1415.77834772171
   (E)  Total one-electron terms..... -3876.12210866648
   (I)  Total two-electron terms.....  1677.31078945486
   (L)  Electronic energy..... -2198.81131921162  (E+I)
```

```
   (N)  Total energy.................  -783.03297148991  (A+L)

 SCFE: SCF energy: HF    -783.03297148991 hartrees   iterations:
5


 HOMO energy:    -0.30239
 LUMO energy:     0.12916

  Orbital energies:
 -20.52749  -15.60024  -11.34678  -11.28597  -11.25620  -11.25012
 -11.24296  -11.24152  -11.24066  -11.23827  -11.23761  -11.23468
 -11.23133  -11.23053  -11.22985  -11.22980  -11.22850  -11.22779
 -11.20925   -1.39681   -1.26922   -1.16533   -1.14927   -1.10629
  -1.03006   -1.01904   -1.01811   -1.01240   -0.96226   -0.93270
  -0.85784   -0.83845   -0.83345   -0.82172   -0.79622   -0.74091
  -0.71135   -0.69495   -0.67351   -0.66430   -0.64398   -0.63837
  -0.62746   -0.61459   -0.61210   -0.60940   -0.59737   -0.58299
  -0.57675   -0.55288   -0.54831   -0.54015   -0.53189   -0.51837
  -0.51531   -0.50739   -0.50074   -0.49807   -0.48493   -0.46840
  -0.46313   -0.42192   -0.41106   -0.34271   -0.33260   -0.32326
  -0.30239    0.12916    0.13421    0.14403    0.15230    0.20371
   0.22963    0.24069    0.24563    0.26192    0.28577

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1      2.504108E-06   5.175930E-05  -1.220436E-04
   2    C1     -2.225581E-05  -5.053871E-04  -2.740533E-04
   3    C2      4.991298E-05   9.875082E-04   7.067818E-04
   4    C3      1.235580E-04  -8.592368E-04  -4.793449E-04
   5    C4     -9.131232E-06   6.978050E-04   1.500731E-04
   6    C5     -9.388585E-05   4.084856E-04  -6.039832E-05
   7    C6      2.839386E-04  -1.296684E-03  -1.261189E-04
   8    C7     -3.880618E-04   6.239050E-04  -4.981213E-04
   9    H3     -8.134166E-05   2.732067E-04  -1.968636E-04
  10    H4      1.114689E-05   3.843725E-04  -6.471063E-06
  11    H6      5.821701E-05  -9.719191E-06   2.547380E-04
```

```
 12    C16    -6.313755E-04  -3.288750E-04   2.792912E-04
 13    C8      1.707411E-03  -5.435318E-04  -3.376603E-04
 14    N2     -1.755000E-04  -2.957523E-03  -3.192080E-03
 15    C9     -7.241573E-04   1.180795E-03   2.136114E-03
 16    C10    -1.127571E-05  -8.951119E-04  -7.563417E-05
 17    O1      1.019333E-04   2.474988E-03  -4.925087E-04
 18    C23     5.891362E-04  -5.699551E-04   7.428124E-04
 19    C18    -1.634850E-04  -3.827278E-04  -4.512226E-04
 20    C19     1.219189E-03  -7.321116E-04  -1.059769E-03
 21    C20     1.261004E-03  -8.011960E-05  -2.577875E-04
 22    C21    -4.437095E-04   1.106407E-03   1.339046E-03
 23    C22    -1.730042E-03   4.828056E-04   3.717746E-04
 24    H2      1.675873E-04   8.494269E-06   5.871413E-05
 25    H5     -8.364469E-05   4.896625E-04   8.008607E-04
 26    H7     -1.912086E-04  -5.163556E-05   4.244774E-05
 27    H8     -2.121368E-05  -3.796039E-04  -6.952036E-04
 28    H9     -1.108485E-04  -7.185916E-05  -1.978142E-04
 29    H10     7.677657E-05   7.279257E-06   1.253114E-04
 30    H19    -1.060459E-03   8.010038E-04   2.658513E-04
 31    H20    -6.437881E-04  -1.572396E-04  -3.268590E-04
 32    H21     3.123074E-04   3.438650E-04  -9.427729E-04
 33    H22    -3.838244E-05  -4.139867E-04   1.056875E-04
 34    H11    -1.071632E-03   9.129954E-04   8.673988E-04
 35    H12     2.574226E-04   2.035965E-04   3.146390E-04
 36    H13     8.062245E-04  -1.155545E-04   1.032341E-03
-----------   -------------  -------------  -------------
   total      -6.671277E-04   1.088073E-03  -1.988441E-04

 end of program der1b


 start of program geopt  12

 geometry optimization step 12
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0377513
  Cos(theta):   0.8098352

  Final level shift:  -8.1398026E-02

 energy change:          -4.5660E-04 .  (  5.0000E-05 )
 gradient maximum:        3.7168E-03 .  (  4.5000E-04 )
 gradient rms:            9.1637E-04 .  (  3.0000E-04 )
 step size:   0.03775  trust radius:   0.03750
 displacement maximum:    1.9221E-02 .  (  1.8000E-03 )
 displacement rms:        3.4178E-03 .  (  1.2000E-03 )
```

```
 predicted energy change:    -2.1272E-04    geom step:   3.7751E-
02    full step:   3.7751E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:     4.0058E-03     y:     1.2459E-03     z:    -2.1634E-03

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1940518699     1.8851648329    -2.2297251280
 C1       -1.1095988722     2.1188908127    -1.1820901870
 C2       -0.8832994453     2.6939962030     1.5038491099
 C3       -0.8867906379     1.0851574978    -0.2874730932
 C4       -1.2156764802     3.4336443853    -0.7585618674
 C5       -1.1010226760     3.7127556348     0.5908523272
 C6       -0.7740809011     1.3743108087     1.0749234290
 C7       -0.7911214007    -0.3528972859    -0.7581620366
 H3       -1.3855816664     4.2219218212    -1.4695876168
 H4       -1.1845658997     4.7248546539     0.9453079489
 H6       -0.8037815150     2.9376627809     2.5448192557
 C16       0.6115475975    -0.7602027662    -1.2088456057
 C8       -1.4003137811    -1.2505344362     0.3413242381
 N2       -0.5264146756     0.3336750773     1.9972837586
 C9       -0.7608481633    -0.9842104684     1.6931655530
 C10       0.0086392301     0.6507271102     3.3147801233
 O1       -0.5128987537    -1.8660309647     2.4643712343
 C23      -1.4041755027    -2.7402927920     0.0170991849
 C18       3.1435287172    -1.5725288680    -2.0824306293
 C19       0.7645153308    -1.4886970369    -2.3833314230
 C20       1.7551610112    -0.4347978966    -0.4838987649
 C21       3.0068126588    -0.8401862801    -0.9138642198
 C22       2.0163547953    -1.8932652332    -2.8187807980
 H2       -0.1037513634    -1.7449165960    -2.9667177726
 H5        1.6752564983     0.1462083250     0.4155641285
 H7        3.8760006692    -0.5796071627    -0.3364314624
 H8        2.1073056630    -2.4569067874    -3.7311017080
 H9        4.1172395122    -1.8849526858    -2.4157651299
 H10      -1.4360254873    -0.4540727475    -1.6243857001
 H19      -0.3987003210    -3.1305017978    -0.0464586848
 H20      -1.9024784854    -2.9133210290    -0.9320302088
 H21      -1.9259285607    -3.2917205349     0.7859806359
 H22      -2.4314879671    -0.9171609465     0.4508030954
 H11       0.9117436350     1.2462227231     3.2196181266
 H12       0.2396808818    -0.2759451348     3.8100816828
 H13      -0.7131821509     1.1947704380     3.9159771581

 nuclear repulsion energy.......  1415.784744570 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  12   /
------------------------------------------------
```

```
  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.330E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     87     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    195    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     96     82
68
  grid # 2      118    118    110    100     91    105     92
78
  grid # 3      224    223    206    194    176    211    176
147
  grid # 4      224    223    207    342    311    390    293
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     71     89     88     88     89     89
71
  grid # 2      122     79     97     95     96     97     96
112
  grid # 3      256    152    183    183    182    184    183
212
  grid # 4      448    290    327    326    327    327    327
211

  number of gridpoints:
```

```
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       70     73     73     73     66     70     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      210    223    223    224    203    217    217
217
  grid # 4      206    223    223    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     71     71   2858
  grid # 2      110    109    106    108   3722
  grid # 3      214    216    214    214   7195
  grid # 4      211    216    207    214   9913

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03248854808           7.2E-05  2.5E-03
etot   2  Y  Y  4  M  -783.03293483029  4.5E-04  2.2E-05  6.3E-04
etot   3  Y  Y  4  M  -783.03298057352  4.6E-05  6.2E-06  1.1E-04
etot   4  Y  Y  4  M  -783.03298388308  3.3E-06  2.8E-06  3.8E-05
etot   5  Y  N  4  M  -783.03298389002  6.9E-09  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.78474457045
   (E)  Total one-electron terms..... -3876.14142059949
   (I)  Total two-electron terms.....  1677.32369213902
   (L)  Electronic energy............. -2198.81772846047  (E+I)
   (N)  Total energy.................  -783.03298389002  (A+L)

 SCFE: SCF energy: HF    -783.03298389002 hartrees   iterations:
5


 HOMO energy:    -0.30204
```

```
LUMO energy:     0.12919

 Orbital energies:
 -20.52677  -15.60047  -11.34587  -11.28609  -11.25654  -11.24988
 -11.24240  -11.24151  -11.24044  -11.23842  -11.23782  -11.23476
 -11.23113  -11.23028  -11.23004  -11.22950  -11.22837  -11.22757
 -11.20844   -1.39829   -1.26971   -1.16516   -1.14889   -1.10620
  -1.03007   -1.01851   -1.01779   -1.01279   -0.96246   -0.93282
  -0.85811   -0.83903   -0.83318   -0.82155   -0.79618   -0.74113
  -0.71139   -0.69485   -0.67342   -0.66425   -0.64423   -0.63810
  -0.62738   -0.61445   -0.61193   -0.60918   -0.59703   -0.58342
  -0.57639   -0.55261   -0.54844   -0.54039   -0.53197   -0.51881
  -0.51507   -0.50735   -0.50075   -0.49791   -0.48473   -0.46855
  -0.46292   -0.42202   -0.41113   -0.34243   -0.33295   -0.32275
  -0.30204    0.12919    0.13422    0.14447    0.15229    0.20453
   0.22986    0.24088    0.24667    0.26167    0.28665

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  14    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
   1     H1    -1.760648E-05   8.560261E-05  -6.701883E-05
   2     C1     5.271573E-05   3.419554E-04   1.900027E-04
   3     C2     1.787746E-04  -7.845456E-05  -1.190407E-04
   4     C3     6.518965E-05   1.733524E-04   2.995630E-05
   5     C4     4.644568E-05  -4.285227E-04  -3.049115E-05
   6     C5     6.634166E-05  -2.814561E-04  -1.310787E-04
   7     C6    -7.423502E-04   6.550684E-04  -5.110122E-04
   8     C7    -1.716607E-05   3.471987E-04   1.017501E-04
   9     H3    -6.693003E-06   1.830384E-05  -5.417540E-05
  10     H4     5.007075E-05   1.713780E-04  -4.002857E-05
  11     H6     3.982523E-05  -1.895296E-04   2.432835E-04
  12     C16   -4.512237E-04   1.458137E-04   2.636271E-04
  13     C8     9.783325E-04  -4.331398E-05  -5.276414E-04
  14     N2     1.154174E-03   1.854764E-03   1.866304E-03
  15     C9    -9.267920E-04   1.908471E-04  -1.722730E-03
  16     C10    2.958805E-04  -1.180492E-04   1.900029E-04
  17     O1     1.093448E-04  -1.675687E-03   1.772626E-03
```

```
 18    C23    -4.258359E-04   5.975215E-04  -2.313616E-04
 19    C18     2.872440E-04  -2.115962E-04  -2.497649E-04
 20    C19    -7.361272E-04   4.485692E-05  -1.675212E-04
 21    C20    -6.108905E-04   2.378031E-04  -4.860949E-05
 22    C21     8.581520E-05   1.631371E-05  -6.928251E-05
 23    C22     3.334914E-04  -3.443841E-04  -3.578032E-04
 24    H2      2.626736E-05   6.559719E-05   1.348223E-04
 25    H5      7.447752E-06   5.255091E-05   2.575070E-04
 26    H7      3.045907E-04   9.256212E-05   1.554336E-04
 27    H8      6.572394E-05   1.325668E-04   6.876751E-05
 28    H9      1.786449E-04  -1.215854E-05  -1.011479E-04
 29    H10    -1.034819E-04  -5.406367E-05  -1.835043E-04
 30    H19     1.116160E-03  -6.221536E-04  -1.694702E-04
 31    H20    -3.862103E-05   1.357032E-04  -2.072739E-04
 32    H21    -5.281330E-04  -3.837875E-04   6.476345E-04
 33    H22    -9.808506E-04   2.228886E-04   1.389144E-04
 34    H11    -1.404782E-03   1.595679E-04  -5.341847E-05
 35    H12     5.411857E-04   1.591068E-04  -1.305233E-04
 36    H13     2.562304E-04  -4.144697E-04  -7.940476E-04
-----------   -------------  -------------  -------------
   total      -7.506569E-04   1.043696E-03   9.368552E-05

 end of program der1b


 start of program geopt  13

 geometry optimization step 13
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0382024
  Cos(theta):   0.6832886

  Final level shift:  -5.3874220E-02

 energy change:          -1.2400E-05 *  (  5.0000E-05 )
 gradient maximum:        2.7846E-03 .  (  4.5000E-04 )
 gradient rms:            5.4966E-04 .  (  3.0000E-04 )
 step size:   0.03820  trust radius:   0.03750
 displacement maximum:    3.0584E-02 .  (  1.8000E-03 )
 displacement rms:        3.4587E-03 .  (  1.2000E-03 )
 predicted energy change:    -1.1855E-04    geom step:   3.8202E-
02    full step:   3.8202E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -2.0794E-03     y:    -6.4346E-04     z:     1.2667E-03
```

new geometry:

atom	x	y	z
		angstroms	
H1	-1.1904634269	1.8837226586	-2.2301003031
C1	-1.1066794715	2.1176325597	-1.1824628321
C2	-0.8810637056	2.6928730351	1.5032217589
C3	-0.8871732520	1.0844565935	-0.2870304827
C4	-1.2097167095	3.4319501345	-0.7595507245
C5	-1.0951751997	3.7113830399	0.5896390562
C6	-0.7750429444	1.3739864102	1.0748917663
C7	-0.7915150688	-0.3538389985	-0.7571326878
H3	-1.3765166026	4.2202553935	-1.4709659876
H4	-1.1757735044	4.7238488899	0.9432542388
H6	-0.8011706181	2.9354752763	2.5444911706
C16	0.6110997752	-0.7603359796	-1.2086064807
C8	-1.4020646732	-1.2508882800	0.3419389292
N2	-0.5250100481	0.3343881834	1.9983400319
C9	-0.7657120961	-0.9851759177	1.6954678759
C10	0.0107116338	0.6544599627	3.3120461746
O1	-0.5273943792	-1.8679756046	2.4703267471
C23	-1.4030490625	-2.7415451131	0.0191963902
C18	3.1453048033	-1.5693529684	-2.0853806533
C19	0.7644423991	-1.4857045768	-2.3849098559
C20	1.7547124057	-0.4376532471	-0.4832782275
C21	3.0072503180	-0.8409531531	-0.9149336996
C22	2.0177736033	-1.8887396774	-2.8217172264
H2	-0.1037812055	-1.7405520052	-2.9690653621
H5	1.6754693014	0.1393394224	0.4183051151
H7	3.8767933085	-0.5805596643	-0.3368344740
H8	2.1089405955	-2.4489979326	-3.7354247468
H9	4.1198020745	-1.8791540814	-2.4195622865
H10	-1.4362030590	-0.4549262882	-1.6239612443
H19	-0.3960516381	-3.1347837625	-0.0355236699
H20	-1.8913092801	-2.9137411212	-0.9351824656
H21	-1.9333958063	-3.2920159127	0.7849544149
H22	-2.4343857842	-0.9175533592	0.4496051989
H11	0.8942234781	1.2760870660	3.2109350826
H12	0.2740813282	-0.2687206992	3.7975013549
H13	-0.7243348673	1.1727815254	3.9195364042

nuclear repulsion energy..... 1415.678442617 hartrees

```
/  end of geometry optimization iteration  13   /
```

end of program geopt

start of program onee
smallest eigenvalue of S: 3.321E-04
number of canonical orbitals.....   368

```
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     87     83
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    195    183    184    189
176
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     96     82
68
  grid # 2      118    118    111    100     90    105     92
79
  grid # 3      223    223    206    194    174    211    176
149
  grid # 4      224    223    206    342    311    390    293
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      256    147    183    182    182    184    183
212
  grid # 4      449    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     70     71
70
  grid # 2      111    118    118    118    106    108    110
108
```

```
  grid # 3      210    222    223    224    202    218    216
217
  grid # 4      206    223    223    224    198    213    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2862
  grid # 2      110    109    107    108   3725
  grid # 3      215    215    213    214   7184
  grid # 4      212    215    209    215   9916

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03273740497           4.5E-05  1.6E-03
etot   2  Y  Y  4  M  -783.03306942744  3.3E-04  2.0E-05  3.8E-04
etot   3  Y  Y  4  M  -783.03311108439  4.2E-05  5.2E-06  7.3E-05
etot   4  Y  Y  4  M  -783.03311138989  3.1E-07  2.3E-06  3.3E-05
etot   5  Y  N  4  M  -783.03311113761 -2.5E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.67844261724
   (E)  Total one-electron terms..... -3875.92480501097
   (I)  Total two-electron terms.....  1677.21325125612
   (L)  Electronic energy............. -2198.71155375485  (E+I)
   (N)  Total energy.................  -783.03311113761  (A+L)

 SCFE: SCF energy: HF    -783.03311113761 hartrees   iterations:
5


 HOMO energy:    -0.30211
 LUMO energy:     0.12921

  Orbital energies:
  -20.52717  -15.60035  -11.34636  -11.28589  -11.25634  -11.24997
  -11.24275  -11.24143  -11.24051  -11.23834  -11.23769  -11.23467
  -11.23125  -11.23043  -11.22988  -11.22966  -11.22845  -11.22764
```

```
 -11.20897   -1.39751   -1.26976   -1.16525   -1.14909   -1.10624
  -1.03008   -1.01880   -1.01795   -1.01258   -0.96252   -0.93273
  -0.85804   -0.83878   -0.83332   -0.82164   -0.79618   -0.74109
  -0.71130   -0.69493   -0.67339   -0.66427   -0.64427   -0.63813
  -0.62740   -0.61458   -0.61219   -0.60914   -0.59731   -0.58318
  -0.57653   -0.55282   -0.54847   -0.54039   -0.53167   -0.51866
  -0.51517   -0.50733   -0.50081   -0.49797   -0.48478   -0.46847
  -0.46300   -0.42185   -0.41134   -0.34259   -0.33276   -0.32300
  -0.30211    0.12921    0.13422    0.14434    0.15237    0.20408
   0.22986    0.24113    0.24685    0.26155    0.28691

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  14    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
   1    H1     -1.288750E-05   5.435393E-05  -6.915185E-05
   2    C1     -1.270972E-05  -1.134496E-04  -1.280113E-04
   3    C2      4.565041E-05   4.981301E-04   3.118425E-04
   4    C3      1.487194E-04  -4.333749E-04  -1.962242E-04
   5    C4      2.397646E-05   2.543932E-04   8.592366E-05
   6    C5     -5.366383E-05   1.385670E-04  -1.135148E-04
   7    C6     -5.265661E-05  -3.668020E-04  -2.917251E-04
   8    C7     -2.753107E-04   4.718202E-04  -1.400342E-04
   9    H3     -5.995114E-05   1.807294E-04  -1.303336E-04
  10    H4      4.300328E-06   2.983533E-04  -5.010494E-06
  11    H6     -5.249997E-05  -1.574786E-05   2.183351E-04
  12    C16    -5.141156E-04  -2.141040E-04   1.718746E-04
  13    C8      1.184320E-03  -2.917670E-04  -3.319124E-04
  14    N2      2.374977E-04  -9.499686E-04  -1.034592E-03
  15    C9     -6.852148E-04   6.227286E-04   3.211726E-04
  16    C10     8.154959E-05  -3.220034E-04   4.358483E-04
  17    O1      9.856838E-05   6.828377E-04   4.590541E-04
  18    C23     5.483586E-05  -6.243503E-05   1.679071E-04
  19    C18     5.125608E-05  -2.397895E-04  -3.112421E-04
  20    C19     3.185482E-04  -2.742615E-04  -5.551371E-04
  21    C20     3.893206E-04   5.978390E-05  -1.267247E-04
  22    C21    -2.013638E-05   5.396529E-04   6.565319E-04
  23    C22    -7.003743E-04   9.383821E-05   1.547313E-05
```

```
 24    H2      1.239858E-04   3.028446E-05   9.172571E-05
 25    H5     -5.439934E-05   2.939706E-04   4.992185E-04
 26    H7     -1.055380E-04  -2.416848E-05   1.226004E-05
 27    H8      1.340910E-05  -1.325221E-04  -3.019458E-04
 28    H9     -3.966028E-05  -3.653435E-05  -1.234830E-04
 29    H10    -4.547557E-06  -5.203934E-05   2.814139E-05
 30    H19    -1.427059E-04   1.767826E-04   5.390872E-05
 31    H20    -2.639856E-04  -8.393821E-05  -1.216691E-04
 32    H21     2.329057E-06   4.590352E-05  -2.741300E-04
 33    H22    -4.149231E-04  -1.137037E-04   4.075030E-05
 34    H11    -9.815653E-04   4.681995E-04   4.081034E-04
 35    H12     2.766771E-04   2.730712E-05   1.832352E-04
 36    H13     6.995641E-04  -2.175200E-04   1.303651E-04
-----------   ------------   ------------   ------------
   total      -6.923372E-04   9.935064E-04   3.682982E-05

 end of program der1b


 start of program geopt  14

 geometry optimization step 14
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0532970
  Cos(theta):   0.5424329

  Final level shift:  -1.3850867E-02

 energy change:          -1.2725E-04 .  (  5.0000E-05 )
 gradient maximum:        2.2112E-03 .  (  4.5000E-04 )
 gradient rms:            4.5911E-04 .  (  3.0000E-04 )
 step size:   0.05330  trust radius:   0.05303
 displacement maximum:    3.6294E-02 .  (  1.8000E-03 )
 displacement rms:        4.8253E-03 .  (  1.2000E-03 )
 predicted energy change:    -9.2975E-05    geom step:   5.3297E-
02    full step:   5.3297E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -4.6025E-04     y:     8.9880E-04     z:    -1.6727E-04

 new geometry:
                                angstroms
 atom            x                  y                  z
 H1       -1.1858989172      1.8823953805     -2.2310924871
 C1       -1.1023287096      2.1168824745     -1.1835552384
```

```
 C2       -0.8773798085      2.6943939687      1.5020790536
 C3       -0.8840206516      1.0838274937     -0.2876189269
 C4       -1.2042939816      3.4322158226     -0.7612013423
 C5       -1.0905585672      3.7127858525      0.5878667040
 C6       -0.7716397891      1.3747586685      1.0739641827
 C7       -0.7902839075     -0.3548906256     -0.7556504696
 H3       -1.3700271509      4.2201565258     -1.4733146737
 H4       -1.1712036334      4.7254640514      0.9408797336
 H6       -0.7994968457      2.9369832158      2.5437009976
 C16       0.6110259546     -0.7620976269     -1.2107522565
 C8       -1.3966602281     -1.2530459526      0.3446899500
 N2       -0.5221651567      0.3364287147      1.9968230459
 C9       -0.7694338271     -0.9813103157      1.7008613088
 C10      -0.0014152885      0.6589938398      3.3174960385
 O1       -0.5416740212     -1.8596146994      2.4828095174
 C23      -1.3885418188     -2.7431231756      0.0237272218
 C18       3.1400549411     -1.5746414088     -2.0925981320
 C19       0.7612605210     -1.4781901303     -2.3930788802
 C20       1.7557691226     -0.4489899506     -0.4817015512
 C21       3.0058965006     -0.8545112205     -0.9159042848
 C22       2.0119544179     -1.8827459131     -2.8327424430
 H2       -0.1079787112     -1.7247145015     -2.9791904316
 H5        1.6773566881      0.1217716771      0.4242774659
 H7        3.8759489061     -0.6040610218     -0.3353159423
 H8        2.1008536305     -2.4366608209     -3.7513274715
 H9        4.1127893494     -1.8871192353     -2.4290017664
 H10      -1.4376049413     -0.4566641571     -1.6200998946
 H19      -0.3802975746     -3.1266325886     -0.0336465554
 H20      -1.8791974112     -2.9213328011     -0.9282401910
 H21      -1.9103793939     -3.2962390061      0.7910739813
 H22      -2.4301103554     -0.9268715573      0.4485818357
 H11       0.8559083364      1.3180954556      3.2271318241
 H12       0.2957714252     -0.2599166806      3.7909355993
 H13      -0.7556085247      1.1405696510      3.9343492359

 nuclear repulsion energy.......  1415.640840664 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  14   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.327E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     87     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     95     82
69
  grid # 2      118    118    111    100     90    104     92
78
  grid # 3      224    223    207    194    175    211    176
147
  grid # 4      224    223    207    342    311    389    292
274

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      256    147    183    183    182    184    183
212
  grid # 4      449    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    217    217
217
  grid # 4      207    223    223    224    197    212    216
215

  number of gridpoints:
```

```
   atom       H22    H11    H12    H13  total
 grid # 1      69     71     70     71   2861
 grid # 2     110    109    106    110   3725
 grid # 3     214    215    213    215   7190
 grid # 4     211    215    210    216   9915

 end of program grid


 start of program rwr
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  2  U  -783.03251762479            8.2E-05  2.5E-03
etot  2  Y  Y  6  M  -783.03322094333  7.0E-04    2.8E-05  6.1E-04
etot  3  Y  Y  6  M  -783.03330682578  8.6E-05    7.9E-06  1.6E-04
etot  4  Y  Y  6  M  -783.03330889700  2.1E-06    2.5E-06  5.3E-05
etot  5  Y  N  6  M  -783.03331126580  2.4E-06    0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.64084066438
   (E)  Total one-electron terms..... -3875.84081947222
   (I)  Total two-electron terms.....  1677.16666754204
   (L)  Electronic energy............. -2198.67415193018  (E+I)
   (N)  Total energy.................  -783.03331126580  (A+L)

 SCFE: SCF energy: HF    -783.03331126580 hartrees   iterations:
5


 HOMO energy:    -0.30193
 LUMO energy:     0.12912

  Orbital energies:
  -20.52691  -15.60058  -11.34609  -11.28593  -11.25677  -11.24985
  -11.24243  -11.24137  -11.24052  -11.23840  -11.23777  -11.23467
  -11.23127  -11.23042  -11.22991  -11.22959  -11.22849  -11.22766
  -11.20837   -1.39820   -1.27031   -1.16527   -1.14902   -1.10636
   -1.03030   -1.01862   -1.01791   -1.01289   -0.96275   -0.93289
   -0.85835   -0.83921   -0.83327   -0.82167   -0.79623   -0.74135
   -0.71145   -0.69500   -0.67335   -0.66438   -0.64448   -0.63795
   -0.62751   -0.61474   -0.61229   -0.60897   -0.59734   -0.58353
   -0.57639   -0.55300   -0.54884   -0.54058   -0.53161   -0.51903
   -0.51510   -0.50742   -0.50095   -0.49792   -0.48477   -0.46865
```

```
 -0.46297   -0.42198   -0.41152   -0.34258   -0.33309   -0.32282
 -0.30193    0.12912    0.13410    0.14454    0.15247    0.20423
  0.22980    0.24117    0.24765    0.26149    0.28750

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -3.524256E-05   1.065608E-04  -8.120840E-05
  2    C1     -1.002020E-05   3.536948E-04   7.481589E-05
  3    C2     -1.246705E-04   2.741715E-04   1.067587E-04
  4    C3     -2.346540E-05   6.013177E-05  -4.006611E-05
  5    C4      6.148821E-05  -2.181700E-04  -1.361860E-04
  6    C5      7.361685E-06  -1.880696E-04  -1.392268E-04
  7    C6     -2.890649E-04   6.032670E-04  -7.223510E-04
  8    C7      1.925499E-04   2.263130E-04  -1.239330E-04
  9    H3     -6.383254E-05   1.447379E-04  -1.380129E-04
 10    H4      1.439763E-05   2.894576E-04  -2.049423E-05
 11    H6     -8.258800E-05  -8.554653E-05   7.233966E-05
 12    C16    -4.568767E-04   1.211172E-04   3.127529E-04
 13    C8      1.134514E-03   3.578829E-05  -7.197385E-04
 14    N2      9.350999E-04   7.759796E-04   1.405185E-03
 15    C9     -5.854298E-04   2.937988E-04  -1.249051E-03
 16    C10    -3.839224E-04   3.042867E-04   5.791023E-04
 17    O1      2.105622E-04  -9.250202E-04   1.534667E-03
 18    C23    -5.711249E-04   4.756442E-04  -3.453687E-04
 19    C18     3.256544E-04  -1.428268E-04  -2.072862E-04
 20    C19    -4.958537E-04   6.243968E-05  -1.122833E-04
 21    C20    -6.533424E-04   1.096493E-04  -2.835288E-04
 22    C21     3.706364E-07  -1.379270E-05  -8.482455E-05
 23    C22     1.820198E-04  -3.416119E-04  -3.971379E-04
 24    H2      4.408484E-05   3.570365E-05   1.189704E-04
 25    H5      2.520549E-05   1.364769E-04   3.601552E-04
 26    H7      3.248830E-04   1.129571E-04   1.503168E-04
 27    H8      7.971610E-05   1.472814E-04   1.381360E-04
 28    H9      1.202347E-04  -1.293464E-05  -9.138707E-05
 29    H10    -5.248024E-05  -1.111912E-04  -1.734442E-04
 30    H19     1.333050E-03  -6.121482E-04  -1.539871E-04
 31    H20    -1.589743E-04   6.037743E-05  -2.377032E-04
```

```
  32    H21    -6.397280E-04  -4.778296E-04   6.001115E-04
  33    H22    -1.475594E-03   2.933252E-04   1.798321E-04
  34    H11    -1.004444E-03  -2.923813E-04   1.362186E-04
  35    H12     5.549843E-04  -3.498955E-05   2.177512E-04
  36    H13     8.037386E-04  -4.785438E-04  -7.619329E-04
 -----------   -------------  -------------  -------------
    total      -7.567395E-04   1.088104E-03  -2.320389E-04

  end of program der1b


  start of program geopt  15

  geometry optimization step 15
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -2.0013E-04 .  (  5.0000E-05 )
  gradient maximum:        1.7505E-03 .  (  4.5000E-04 )
  gradient rms:            4.5754E-04 .  (  3.0000E-04 )
  step size:   0.08665  trust radius:   0.10607
  displacement maximum:    4.4982E-02 .  (  1.8000E-03 )
  displacement rms:        7.8450E-03 .  (  1.2000E-03 )
  predicted energy change:    -7.7739E-05    geom step:   8.6650E-
02    full step:   8.6650E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -4.7965E-03     y:    -4.8356E-04     z:     2.2999E-03

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1947650016     1.8846951347    -2.2330885775
  C1       -1.1087416111     2.1179993868    -1.1856597580
  C2       -0.8787134484     2.6922588809     1.5006721766
  C3       -0.8846920120     1.0848907600    -0.2913257755
  C4       -1.2133860416     3.4317947326    -0.7613572263
  C5       -1.0975293825     3.7108456748     0.5880048523
  C6       -0.7687767697     1.3745596098     1.0700894203
  C7       -0.7893167406    -0.3546127641    -0.7582648748
  H3       -1.3836003561     4.2205567876    -1.4717710497
  H4       -1.1811327300     4.7229998441     0.9422492244
  H6       -0.7989811603     2.9311513680     2.5428786033
  C16       0.6134578700    -0.7634358285    -1.2074962212
  C8       -1.4032877799    -1.2498338118     0.3409889096
  N2       -0.5078409029     0.3357566671     1.9919926211
  C9       -0.7807122882    -0.9807390908     1.7005554219
  C10       0.0363180228     0.6576292576     3.2987926101
```

```
  O1       -0.5743741091     -1.8598938873      2.4887626630
  C23      -1.3997664177     -2.7421100708      0.0222447399
  C18       3.1484722001     -1.5723422298     -2.0830281511
  C19       0.7694595113     -1.4735735464     -2.3922512805
  C20       1.7550676876     -0.4563967549     -0.4724310966
  C21       3.0078739799     -0.8583779813     -0.9041994549
  C22       2.0229502197     -1.8779138473     -2.8278423723
  H2       -0.0969454377     -1.7159769702     -2.9839038874
  H5        1.6744376545      0.1064845295      0.4378534042
  H7        3.8757890200     -0.6084339448     -0.3196830722
  H8        2.1157494955     -2.4289756257     -3.7466138553
  H9        4.1231766981     -1.8822373567     -2.4164187747
  H10      -1.4326628505     -0.4568257177     -1.6259204194
  H19      -0.3906823217     -3.1437814798      0.0078673786
  H20      -1.8525325938     -2.9112697222     -0.9506604585
  H21      -1.9632378318     -3.2882310144      0.7703686903
  H22      -2.4377402215     -0.9173243063      0.4398843384
  H11       0.8651469715      1.3471861789      3.1895865438
  H12       0.3804648060     -0.2531034612      3.7575719169
  H13      -0.7211811637      1.1081418111      3.9329544075

  nuclear repulsion energy.......  1415.483964889 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  15   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.326E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     87     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    195    183    184    189
176
  grid # 4      216    326    328    338    328    328    323
314
```

```
  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     96     82
69
  grid # 2      118    118    111    100     90    106     92
78
  grid # 3      224    223    207    194    173    210    176
147
  grid # 4      224    223    207    342    310    388    294
274

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     71     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    152    183    182    182    184    183
212
  grid # 4      450    290    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     70     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    222    223    224    202    218    216
217
  grid # 4      207    223    223    224    198    216    217
217

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2859
  grid # 2      110    109    107    111   3727
  grid # 3      215    214    213    215   7190
  grid # 4      212    211    209    216   9921

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf
```

```
       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  2  U  -783.03161533907           9.0E-05  2.4E-03
etot   2  Y  Y  6  M  -783.03309043745  1.5E-03  4.0E-05  6.7E-04
etot   3  Y  Y  6  M  -783.03326038684  1.7E-04  1.0E-05  1.3E-04
etot   4  Y  Y  6  M  -783.03326773551  7.3E-06  3.9E-06  6.6E-05
etot   5  Y  N  6  M  -783.03326817214  4.4E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.48396488863
   (E)  Total one-electron terms..... -3875.52541748963
   (I)  Total two-electron terms.....  1677.00818442886
   (L)  Electronic energy............. -2198.51723306077  (E+I)
   (N)  Total energy.................  -783.03326817214  (A+L)

 SCFE: SCF energy: HF    -783.03326817214 hartrees   iterations:
5


 HOMO energy:    -0.30229
 LUMO energy:     0.12914

  Orbital energies:
  -20.52702  -15.60027  -11.34640  -11.28583  -11.25665  -11.25004
  -11.24314  -11.24163  -11.24052  -11.23853  -11.23785  -11.23484
  -11.23125  -11.23045  -11.23011  -11.22964  -11.22847  -11.22760
  -11.21011   -1.39730   -1.27012   -1.16533   -1.14926   -1.10618
   -1.02997   -1.01891   -1.01815   -1.01268   -0.96285   -0.93251
   -0.85795   -0.83875   -0.83343   -0.82178   -0.79625   -0.74117
   -0.71123   -0.69516   -0.67309   -0.66439   -0.64470   -0.63804
   -0.62741   -0.61499   -0.61246   -0.60880   -0.59753   -0.58321
   -0.57644   -0.55346   -0.54873   -0.54033   -0.53117   -0.51881
   -0.51521   -0.50715   -0.50107   -0.49810   -0.48474   -0.46850
   -0.46296   -0.42137   -0.41143   -0.34267   -0.33290   -0.32324
   -0.30229    0.12914    0.13395    0.14463    0.15254    0.20366
    0.22918    0.24097    0.24745    0.26140    0.28684

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr
```

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	-3.060099E-05	3.708702E-05	-2.018024E-04
2	C1	-4.311779E-05	-2.841001E-04	-5.547012E-05
3	C2	-1.113699E-04	3.844960E-04	-3.879661E-05
4	C3	1.529154E-04	-6.530408E-04	1.003069E-04
5	C4	-5.784681E-06	4.597214E-04	2.375900E-04
6	C5	-6.483505E-05	2.557698E-04	-1.597196E-05
7	C6	5.383050E-04	-1.062592E-04	-5.595230E-05
8	C7	4.348823E-05	2.598916E-04	-7.173185E-05
9	H3	-2.164322E-05	5.967583E-05	-5.931434E-05
10	H4	1.982270E-05	2.157185E-04	-4.382692E-05
11	H6	-1.841104E-04	2.547983E-04	1.830271E-04
12	C16	-6.266728E-04	-2.618815E-05	3.097450E-04
13	C8	4.527106E-04	2.936681E-04	-2.955051E-04
14	N2	-7.106531E-04	-2.465873E-03	-4.131084E-03
15	C9	4.788254E-05	1.028947E-03	7.484797E-04
16	C10	-9.073112E-04	4.252671E-04	1.611055E-03
17	O1	4.333538E-04	9.887816E-04	5.242424E-04
18	C23	1.198317E-03	-1.220785E-03	8.994733E-04
19	C18	2.659446E-05	-3.318956E-04	-3.791696E-04
20	C19	3.462801E-04	-4.931917E-04	-6.328651E-04
21	C20	6.884813E-04	1.563060E-04	7.072406E-05
22	C21	-1.662681E-04	5.812758E-04	7.013171E-04
23	C22	-7.373702E-04	1.394381E-04	1.009011E-04
24	H2	-9.917171E-06	-9.172417E-05	-4.217731E-05
25	H5	-9.875964E-05	4.064711E-04	4.152519E-04
26	H7	7.159916E-05	-2.086328E-06	2.214453E-04
27	H8	-8.883540E-06	-1.398107E-04	-5.794112E-04
28	H9	-2.205235E-05	-4.751086E-05	-1.550688E-04
29	H10	-2.087770E-05	-5.904105E-05	3.611627E-06
30	H19	-2.512526E-03	1.359009E-03	-2.015217E-04
31	H20	-1.071527E-04	-4.546762E-04	4.436451E-04
32	H21	8.155298E-04	7.496449E-04	-1.389169E-03
33	H22	-1.009438E-05	-4.959373E-04	-2.913758E-05
34	H11	-2.132448E-04	1.610149E-04	5.109761E-04
35	H12	-1.745427E-04	-8.165475E-05	1.852349E-06
36	H13	1.207053E-03	-1.820410E-04	1.163118E-03
total		-7.454553E-04	1.081166E-03	-1.312139E-04

end of program der1b

start of program geopt 16

geometry optimization step 16

```
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  ** restarting optimization from step   15 **


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0531195
   Cos(theta):   0.4412467

   Final level shift:  -8.1156573E-03

  energy change:           4.3094E-05 *  (  5.0000E-05 )
  gradient maximum:        1.7505E-03 .  (  4.5000E-04 )
  gradient rms:            4.5754E-04 .  (  3.0000E-04 )
  step size:   0.05312  trust radius:   0.05303
  displacement maximum:    2.7120E-02 .  (  1.8000E-03 )
  displacement rms:        4.8092E-03 .  (  1.2000E-03 )
  predicted energy change:    -7.0676E-05    geom step:   5.3119E-
02    full step:   5.3119E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.9837E-16     y:     6.2450E-17     z:    -1.2490E-16

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1918354972     1.8851439646    -2.2311448599
  C1       -1.1067318143     2.1183362401    -1.1835425870
  C2       -0.8792060913     2.6928433636     1.5028139846
  C3       -0.8855034501     1.0847856018    -0.2889095130
  C4       -1.2098149278     3.4325475328    -0.7597725072
  C5       -1.0950547607     3.7116657231     0.5896242435
  C6       -0.7709958352     1.3745005316     1.0727816603
  C7       -0.7907781251    -0.3544011243    -0.7570474495
  H3       -1.3779914135     4.2212665374    -1.4706877572
  H4       -1.1771194540     4.7241372853     0.9434529247
  H6       -0.8008946019     2.9325991890     2.5449204145
  C16       0.6111714616    -0.7629762330    -1.2084682675
  C8       -1.4028293727    -1.2508155236     0.3422347949
  N2       -0.5138162728     0.3351427840     1.9950237512
  C9       -0.7772018313    -0.9820928136     1.7006681560
  C10       0.0185526492     0.6557343718     3.3087592086
  O1       -0.5628018410    -1.8614977692     2.4864620596
  C23      -1.3997187314    -2.7428695130     0.0225933957
  C18       3.1448844348    -1.5726637657    -2.0866352002
  C19       0.7648229441    -1.4810102200    -2.3888740259
  C20       1.7544718645    -0.4479391704    -0.4794694902
  C21       3.0066768432    -0.8508198363    -0.9122519585
  C22       2.0176636311    -1.8852177753    -2.8260196663
```

```
  H2       -0.1029720049     -1.7293142820     -2.9758849564
  H5        1.6755312709      0.1223272367      0.4266605439
  H7        3.8760334472     -0.5954840883     -0.3319392705
  H8        2.1089427219     -2.4410159997     -3.7419681917
  H9        4.1191110472     -1.8827663261     -2.4212186301
  H10      -1.4353734703     -0.4563109657     -1.6237184925
  H19      -0.3907057866     -3.1397667494     -0.0101394135
  H20      -1.8683647284     -2.9143115262     -0.9420969431
  H21      -1.9483838333     -3.2911924180      0.7787257918
  H22      -2.4375056292     -0.9192875464      0.4437870735
  H11       0.8575753176      1.3345383445      3.2085717012
  H12       0.3459123929     -0.2581712247      3.7734700424
  H13      -0.7393600084      1.1167054187      3.9344542823

  nuclear repulsion energy.......  1415.353750309 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  16   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.328E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     87     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    195    183    184    189
176
  grid # 4      216    326    328    338    328    328    323
313

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     96     82
69
```

```
  grid # 2      118    118    111    100     90    105     92
78
  grid # 3      224    223    207    194    173    210    176
147
  grid # 4      224    223    207    342    311    389    294
274

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      256    150    183    182    182    184    183
212
  grid # 4      450    290    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     70     71
70
  grid # 2      111    118    118    118    106    109    110
108
  grid # 3      211    222    223    224    202    218    216
217
  grid # 4      207    223    223    224    196    215    216
216

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2862
  grid # 2      110    109    107    111   3728
  grid # 3      215    214    212    215   7185
  grid # 4      212    213    210    216   9920

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error
```

```
etot   1  N  N  1  U  -783.03281706934           5.0E-05  1.4E-03
etot   2  Y  Y  4  M  -783.03312427828  3.1E-04  1.9E-05  5.8E-04
etot   3  Y  Y  4  M  -783.03316288335  3.9E-05  5.4E-06  1.4E-04
etot   4  Y  Y  4  M  -783.03316539364  2.5E-06  1.4E-06  3.9E-05
etot   5  Y  N  4  M  -783.03316407596 -1.3E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.35375030938
   (E)  Total one-electron terms..... -3875.27441835414
   (I)  Total two-electron terms.....  1676.88750396881
   (L)  Electronic energy............. -2198.38691438533  (E+I)
   (N)  Total energy.................  -783.03316407596  (A+L)

 SCFE: SCF energy: HF    -783.03316407596 hartrees   iterations:
5


 HOMO energy:    -0.30213
 LUMO energy:     0.12924

  Orbital energies:
  -20.52707  -15.60020  -11.34629  -11.28584  -11.25652  -11.25000
  -11.24311  -11.24157  -11.24048  -11.23852  -11.23784  -11.23476
  -11.23123  -11.23035  -11.23007  -11.22964  -11.22841  -11.22751
  -11.20968   -1.39733   -1.26979   -1.16525   -1.14913   -1.10610
   -1.02995   -1.01878   -1.01805   -1.01260   -0.96266   -0.93258
   -0.85795   -0.83875   -0.83336   -0.82170   -0.79617   -0.74108
   -0.71115   -0.69504   -0.67310   -0.66427   -0.64450   -0.63793
   -0.62738   -0.61482   -0.61232   -0.60880   -0.59731   -0.58316
   -0.57644   -0.55320   -0.54867   -0.54041   -0.53126   -0.51874
   -0.51508   -0.50717   -0.50099   -0.49797   -0.48466   -0.46850
   -0.46293   -0.42148   -0.41144   -0.34262   -0.33281   -0.32311
   -0.30213    0.12924    0.13409    0.14454    0.15246    0.20386
    0.22952    0.24093    0.24768    0.26140    0.28713

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x             y             z
```

1	H1	-2.076901E-05	2.725807E-05	-1.228720E-04
2	C1	-5.423186E-05	-1.729491E-04	-8.691033E-05
3	C2	-1.289445E-04	2.879280E-04	-4.350675E-05
4	C3	1.646959E-04	-4.729124E-04	5.380076E-05
5	C4	-1.950331E-06	2.805998E-04	2.022463E-04
6	C5	-6.353908E-05	1.930004E-04	-4.295208E-05
7	C6	4.111472E-04	-1.519043E-04	1.292671E-06
8	C7	-1.199114E-04	2.088626E-04	-7.096114E-05
9	H3	-1.733939E-05	5.333553E-05	-4.289213E-05
10	H4	8.980717E-06	1.512606E-04	-2.857306E-05
11	H6	-9.930237E-05	1.531849E-04	1.835794E-04
12	C16	-4.761430E-04	4.800321E-06	2.702735E-04
13	C8	4.171914E-04	6.556764E-05	-1.226432E-04
14	N2	-3.654317E-04	-1.685129E-03	-2.606026E-03
15	C9	-2.346116E-04	6.838593E-04	4.703105E-04
16	C10	-4.320746E-04	2.530715E-04	8.913516E-04
17	O1	2.084272E-04	8.071311E-04	3.461610E-04
18	C23	7.889505E-04	-6.377477E-04	4.817368E-04
19	C18	4.065821E-05	-2.771372E-04	-3.579461E-04
20	C19	2.773252E-04	-3.657966E-04	-5.634945E-04
21	C20	6.175470E-04	2.045268E-04	1.886286E-04
22	C21	-4.261402E-05	5.302141E-04	7.127327E-04
23	C22	-6.735100E-04	1.901480E-04	1.651498E-04
24	H2	-3.931484E-05	-7.049288E-05	-6.962124E-05
25	H5	-8.499968E-05	2.469456E-04	3.083788E-04
26	H7	-1.678894E-05	-9.138450E-06	1.410601E-04
27	H8	-2.266994E-05	-2.188366E-04	-5.946609E-04
28	H9	-1.935856E-05	-3.802608E-05	-1.345884E-04
29	H10	-4.593859E-05	-9.718123E-07	-2.735757E-05
30	H19	-1.645610E-03	8.687701E-04	-2.585829E-06
31	H20	-1.278384E-04	-2.684396E-04	1.942621E-04
32	H21	5.471564E-04	5.037196E-04	-8.970119E-04
33	H22	1.637880E-04	-4.152862E-04	-7.264908E-06
34	H11	-3.232297E-04	1.945023E-04	3.963368E-04
35	H12	-9.372187E-05	5.768344E-05	-1.361023E-04
36	H13	7.823837E-04	-1.474820E-04	7.571220E-04
total		-7.215922E-04	1.034119E-03	-1.935473E-04

```
 end of program der1b


 start of program geopt  17

 geometry optimization step 17
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
```

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0265807
   Cos(theta):   0.7409701

   Final level shift:  -6.8506355E-02

  energy change:           1.4719E-04 .  (  5.0000E-05 )
  gradient maximum:        2.2248E-03 .  (  4.5000E-04 )
  gradient rms:            5.5697E-04 .  (  3.0000E-04 )
  step size:   0.02658  trust radius:   0.02652
  displacement maximum:    1.0933E-02 .  (  1.8000E-03 )
  displacement rms:        2.4065E-03 .  (  1.2000E-03 )
  predicted energy change:    -8.4783E-05    geom step:   2.6581E-
02    full step:   2.6581E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     2.3817E-03     y:     1.2274E-03     z:    -1.1433E-03

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -1.1898670125      1.8847814228     -2.2312119782
  C1       -1.1048480005      2.1182799966     -1.1835504621
  C2       -0.8792107212      2.6947980897      1.5025377048
  C3       -0.8827653820      1.0849454487     -0.2887521400
  C4       -1.2089879760      3.4331824117     -0.7602007013
  C5       -1.0957139377      3.7132983564      0.5889335586
  C6       -0.7682447348      1.3759218048      1.0725986528
  C7       -0.7891365630     -0.3542605682     -0.7561911903
  H3       -1.3775548433      4.2212046348     -1.4717432801
  H4       -1.1793645619      4.7258673145      0.9422053341
  H6       -0.8034265487      2.9353933583      2.5448972832
  C16       0.6116893955     -0.7637076923     -1.2098042482
  C8       -1.3978045847     -1.2513065921      0.3442611398
  N2       -0.5134715743      0.3366800036      1.9935604050
  C9       -0.7743495947     -0.9791894005      1.7027239833
  C10       0.0027490065      0.6561503639      3.3175421975
  O1       -0.5582315656     -1.8549797778      2.4912389243
  C23      -1.3925212087     -2.7422485199      0.0239800314
  C18       3.1402859060     -1.5785644872     -2.0922965546
  C19       0.7615386908     -1.4807666283     -2.3917699342
  C20       1.7568427781     -0.4512066930     -0.4810174519
  C21       3.0067390273     -0.8575492804     -0.9157727903
  C22       2.0116680474     -1.8867295727     -2.8315168956
  H2       -0.1078201647     -1.7272925271     -2.9774653816
  H5        1.6791443781      0.1188975757      0.4256616758
  H7        3.8772712996     -0.6070442980     -0.3355749421
  H8        2.1002122184     -2.4410169802     -3.7497844214
  H9        4.1125970487     -1.8917450250     -2.4292892256
  H10      -1.4355993333     -0.4565516128     -1.6212464322
  H19      -0.3849360709     -3.1307458989     -0.0207071702
```

```
  H20      -1.8736487576     -2.9188298705     -0.9334269167
  H21      -1.9267703492     -3.2927445472      0.7851494854
  H22      -2.4324876488     -0.9244628370      0.4464388908
  H11       0.8360800064      1.3443455025      3.2328270212
  H12       0.3325143945     -0.2588686433      3.7779313019
  H13      -0.7615532962      1.1050320069      3.9458298010

  nuclear repulsion energy.......  1415.297894215 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  17   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.331E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     87     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    325
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     71     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
145
  grid # 4      224    223    207    342    311    388    294
277

  number of gridpoints:
```

```
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     71     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      256    152    183    183    182    184    183
212
  grid # 4      449    288    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    217
217
  grid # 4      207    223    223    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2859
  grid # 2      110    109    106    111   3728
  grid # 3      214    215    212    215   7190
  grid # 4      211    213    210    217   9919

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS     maximum
       t  p  i  c  r                              energy   density    DIIS
       e  d  i  u  i                total energy  change   change     error

etot   1  N  N  1  U  -783.03300183202            3.3E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03318587615  1.8E-04   1.4E-05  3.4E-04
etot   3  Y  Y  4  M  -783.03320331669  1.7E-05   3.9E-06  6.2E-05
etot   4  Y  N  4  M  -783.03320434631  1.0E-06   0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.29789421495
```

```
   (E)  Total one-electron terms..... -3875.16241680966
   (I)  Total two-electron terms.....  1676.83131824839
   (L)  Electronic energy............ -2198.33109856126  (E+I)
   (N)  Total energy.................  -783.03320434631  (A+L)

 SCFE: SCF energy: HF    -783.03320434631 hartrees   iterations:
4


 HOMO energy:    -0.30197
 LUMO energy:     0.12921

  Orbital energies:
 -20.52684  -15.60050  -11.34590  -11.28604  -11.25678  -11.24987
 -11.24264  -11.24147  -11.24048  -11.23849  -11.23785  -11.23492
 -11.23111  -11.23050  -11.22996  -11.22944  -11.22849  -11.22768
 -11.20864   -1.39792   -1.26998   -1.16512   -1.14897   -1.10614
  -1.03014   -1.01860   -1.01784   -1.01281   -0.96266   -0.93281
  -0.85828   -0.83916   -0.83325   -0.82164   -0.79616   -0.74127
  -0.71120   -0.69498   -0.67312   -0.66430   -0.64456   -0.63769
  -0.62742   -0.61478   -0.61221   -0.60866   -0.59705   -0.58341
  -0.57631   -0.55306   -0.54889   -0.54060   -0.53132   -0.51912
  -0.51501   -0.50728   -0.50098   -0.49785   -0.48462   -0.46862
  -0.46285   -0.42179   -0.41154   -0.34254   -0.33299   -0.32282
  -0.30197    0.12921    0.13407    0.14466    0.15242    0.20419
   0.22970    0.24107    0.24826    0.26133    0.28773

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x             y             z
 ----  -----   -------------  -------------  -------------
   1    H1     -2.749844E-05   5.927659E-05  -5.814880E-05
   2    C1      6.598569E-06   2.269102E-04  -1.976546E-05
   3    C2     -4.731144E-05  -8.456915E-05  -7.424503E-05
   4    C3      6.844551E-05   1.050694E-04  -3.747773E-05
   5    C4     -1.899668E-05  -2.254398E-04  -1.838663E-04
   6    C5      6.886463E-05  -1.041397E-04   1.057060E-04
   7    C6     -3.347210E-04   6.361344E-04  -3.336204E-04
   8    C7      8.620343E-05   1.500224E-04   1.421189E-04
```

```
 9    H3     -2.416687E-05   7.394918E-05  -7.900144E-05
10    H4      1.012906E-05   1.174894E-04  -1.772366E-05
11    H6     -5.179638E-05  -3.655656E-05   2.603832E-05
12    C16    -1.708505E-04   1.283013E-04   2.149589E-04
13    C8      2.502808E-04   2.741050E-05  -4.545473E-04
14    N2      6.186347E-04   1.056552E-03   1.747326E-03
15    C9     -2.667254E-04  -1.173440E-04  -1.132280E-03
16    C10    -3.181214E-04   2.014716E-04   3.956910E-04
17    O1     -7.694118E-05  -8.723296E-04   8.358388E-04
18    C23    -3.467583E-04   4.299200E-04  -1.072602E-04
19    C18     2.690961E-04   1.706250E-05   4.513839E-05
20    C19    -5.980987E-04   8.338675E-05   1.522454E-05
21    C20    -4.635482E-04   4.868756E-05  -2.228858E-04
22    C21     4.446269E-06  -6.936987E-05  -1.304250E-04
23    C22     3.078131E-04  -2.578838E-04  -3.481255E-04
24    H2     -5.730636E-05   4.950621E-05   4.405165E-05
25    H5      1.954477E-05   8.568029E-05   1.362704E-04
26    H7      1.955898E-04   6.536586E-05   6.807380E-05
27    H8      2.136577E-05   8.484329E-05   6.902984E-05
28    H9      1.176141E-04   2.350077E-05  -3.718630E-05
29    H10    -7.745929E-05  -1.919398E-05  -1.077771E-04
30    H19     9.168477E-04  -4.872536E-04  -2.307688E-04
31    H20     4.162644E-05   1.152786E-04  -1.060391E-04
32    H21    -4.315960E-04  -2.893514E-04   5.597398E-04
33    H22    -6.949958E-04   1.913902E-04   6.240169E-05
34    H11    -3.837703E-04  -2.583737E-04  -1.603510E-04
35    H12     3.527341E-04   2.183684E-04  -1.301972E-04
36    H13     2.763897E-04  -3.265669E-04  -6.912106E-04
-----------   -------------  -------------  -------------
  total      -7.584374E-04   1.047206E-03  -1.952950E-04

 end of program der1b


 start of program geopt  18

 geometry optimization step 18
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0137363
  Cos(theta):   0.8065497

  Final level shift:  -8.3596499E-02

 energy change:          -4.0270E-05 *  (  5.0000E-05 )
 gradient maximum:        1.2883E-03 .  (  4.5000E-04 )
 gradient rms:            3.2139E-04 .  (  3.0000E-04 )
```

```
  step size:   0.01374  trust radius:   0.01326
  displacement maximum:    6.6985E-03 .  (  1.8000E-03 )
  displacement rms:        1.2436E-03 .  (  1.2000E-03 )
  predicted energy change:    -2.7552E-05    geom step:   1.3736E-
02    full step:   1.3736E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.5235E-03     y:    -4.0647E-04     z:     7.4771E-04

  new geometry:
                                angstroms
  atom            x                 y                 z
  H1       -1.1873201905      1.8847634922     -2.2316677566
  C1       -1.1030927878      2.1181482941     -1.1838949647
  C2       -0.8793751125      2.6942968872      1.5026495827
  C3       -0.8831297266      1.0848371531     -0.2886072788
  C4       -1.2059743721      3.4328132344     -0.7606814381
  C5       -1.0935475219      3.7128224899      0.5887436011
  C6       -0.7695904075      1.3757737576      1.0729413905
  C7       -0.7894824952     -0.3544991003     -0.7560809962
  H3       -1.3727172012      4.2211109616     -1.4723735491
  H4       -1.1760485333      4.7256364509      0.9416702526
  H6       -0.8043688305      2.9342827658      2.5452018449
  C16       0.6114086448     -0.7638246990     -1.2093397432
  C8       -1.3998887338     -1.2513678609      0.3434764623
  N2       -0.5138422878      0.3364061235      1.9950808208
  C9       -0.7771007553     -0.9804147754      1.7027745446
  C10       0.0072741871      0.6564495426      3.3154525576
  O1       -0.5651632382     -1.8573120923      2.4922138261
  C23      -1.3936276975     -2.7431444845      0.0243600060
  C18       3.1422273541     -1.5758415904     -2.0922880672
  C19       0.7620756166     -1.4811102087     -2.3911003006
  C20       1.7562864098     -0.4502741568     -0.4813537730
  C21       3.0071222281     -0.8549068134     -0.9162439280
  C22       2.0135734768     -1.8859168373     -2.8309234675
  H2       -0.1070555713     -1.7282159956     -2.9767969015
  H5        1.6788163286      0.1199897869      0.4253120691
  H7        3.8777025726     -0.6024257981     -0.3363393376
  H8        2.1028749005     -2.4399435875     -3.7487532009
  H9        4.1154148838     -1.8870620979     -2.4291195615
  H10      -1.4352711356     -0.4565037202     -1.6219412074
  H19      -0.3849834116     -3.1343619628     -0.0163225673
  H20      -1.8697367307     -2.9191031173     -0.9356050868
  H21      -1.9328123769     -3.2927915575      0.7844882831
  H22      -2.4355094942     -0.9238968046      0.4447369194
  H11       0.8369736876      1.3475962853      3.2248941067
  H12       0.3453110102     -0.2566078447      3.7735528480
  H13      -0.7573821029      1.1013079917      3.9446352106

  nuclear repulsion energy.......  1415.142182431 hartrees
  ------------------------------------------------
```

```
 /  end of geometry optimization iteration  18   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.330E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    195    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
147
  grid # 4      224    223    207    342    311    388    294
274

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      256    148    183    183    182    184    183
212
```

```
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    213    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2862
  grid # 2      110    109    107    111   3728
  grid # 3      215    215    212    215   7189
  grid # 4      211    211    209    217   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03316813319           1.7E-05  3.6E-04
etot   2  Y  Y  4  M  -783.03320871235  4.1E-05  6.7E-06  1.0E-04
etot   3  Y  Y  4  M  -783.03321401475  5.3E-06  2.1E-06  3.4E-05
etot   4  Y  N  4  M  -783.03321493573  9.2E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.14218243080
   (E)  Total one-electron terms..... -3874.85345685298
   (I)  Total two-electron terms.....  1676.67805948645
   (L)  Electronic energy............. -2198.17539736653  (E+I)
   (N)  Total energy.................  -783.03321493573  (A+L)

 SCFE: SCF energy: HF    -783.03321493573 hartrees   iterations:
4
```

```
HOMO energy:    -0.30201
LUMO energy:     0.12921


 Orbital energies:
 -20.52697  -15.60038  -11.34624  -11.28588  -11.25650  -11.24994
 -11.24304  -11.24148  -11.24048  -11.23855  -11.23785  -11.23475
 -11.23134  -11.23048  -11.23004  -11.22972  -11.22853  -11.22759
 -11.20919   -1.39736   -1.26963   -1.16513   -1.14900   -1.10610
  -1.03006   -1.01867   -1.01790   -1.01264   -0.96261   -0.93271
  -0.85811   -0.83887   -0.83329   -0.82166   -0.79611   -0.74110
  -0.71110   -0.69497   -0.67302   -0.66425   -0.64448   -0.63774
  -0.62740   -0.61479   -0.61224   -0.60871   -0.59714   -0.58325
  -0.57639   -0.55316   -0.54871   -0.54057   -0.53120   -0.51893
  -0.51499   -0.50724   -0.50096   -0.49785   -0.48463   -0.46858
  -0.46290   -0.42160   -0.41153   -0.34260   -0.33286   -0.32296
  -0.30201    0.12921    0.13408    0.14452    0.15240    0.20389
   0.22965    0.24098    0.24815    0.26134    0.28753

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -1.960124E-05   3.371344E-05  -1.950939E-05
  2    C1     -2.780475E-05   2.698006E-05  -6.631887E-05
  3    C2     -1.058196E-04   1.824795E-04   8.711571E-05
  4    C3      1.271265E-04  -1.601169E-04   2.538795E-05
  5    C4     -1.181164E-05   1.228740E-04   7.946300E-05
  6    C5     -3.370351E-05   1.238149E-04  -1.371151E-04
  7    C6      1.719533E-04  -2.059000E-04  -6.253616E-05
  8    C7     -1.798474E-04   1.730538E-04  -6.963155E-05
  9    H3     -3.587927E-05   6.386988E-05  -4.286803E-05
 10    H4     -1.591673E-05   8.250113E-05  -1.339744E-05
 11    H6     -5.723768E-05   5.968289E-05   3.704330E-05
 12    C16    -2.046426E-04  -5.050863E-05  -1.129473E-05
 13    C8      2.966512E-04  -1.082374E-04  -1.092849E-04
 14    N2     -4.061630E-05  -4.460462E-04  -6.972469E-04
 15    C9     -2.582695E-04   2.833889E-04   4.096679E-04
```

```
 16    C10    -1.705919E-04  -5.459403E-05   1.824871E-04
 17    O1      3.662036E-05   4.738231E-04  -4.832017E-05
 18    C23     1.187420E-04  -9.212490E-05   2.147317E-04
 19    C18     7.896305E-06  -1.099049E-04  -1.474924E-04
 20    C19     2.015475E-04  -1.105140E-04  -2.052264E-04
 21    C20     1.795557E-04   1.530909E-04   5.118744E-05
 22    C21     3.191963E-05   1.906495E-04   2.865419E-04
 23    C22    -3.622568E-04   1.292405E-04   5.921281E-05
 24    H2     -8.805562E-06  -1.154540E-07   2.095742E-06
 25    H5     -4.188889E-05   8.434437E-05   1.262667E-04
 26    H7     -4.647847E-05   3.847366E-06   2.402106E-05
 27    H8     -1.568541E-05  -7.199004E-05  -2.011127E-04
 28    H9     -4.583838E-05   2.139176E-06  -4.374302E-05
 29    H10    -1.615027E-05   2.261342E-05   2.086467E-05
 30    H19    -2.411518E-04   1.881472E-04  -5.995746E-05
 31    H20    -1.282477E-04  -2.487653E-05  -4.113130E-05
 32    H21     8.497377E-05   1.055472E-04  -1.989192E-04
 33    H22    -2.420652E-05  -9.758595E-05   3.071754E-06
 34    H11    -2.389571E-04   1.149375E-04   1.402976E-04
 35    H12     7.763427E-05   1.386311E-05   2.537519E-05
 36    H13     2.765265E-04  -7.334709E-05   1.762824E-04
-----------   -------------  -------------  -------------
   total      -7.202619E-04   1.028740E-03  -2.239920E-04

 end of program der1b


 start of program geopt  19

 geometry optimization step 19
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0101697
  Cos(theta):   0.7144539

  Final level shift:  -6.5682809E-02

 energy change:          -1.0589E-05 *  (  5.0000E-05 )
 gradient maximum:        8.7892E-04 .  (  4.5000E-04 )
 gradient rms:            2.1682E-04 *  (  3.0000E-04 )
 step size:   0.01017  trust radius:   0.01000
 displacement maximum:    4.2088E-03 .  (  1.8000E-03 )
 displacement rms:        9.2072E-04 *  (  1.2000E-03 )
 predicted energy change:    -1.2097E-05    geom step:   1.0170E-
02    full step:   1.0170E-02
 molecular structure not yet converged...
```

```
 center of mass moved by:
    x:     8.7882E-04     y:     5.6513E-04     z:    -4.1137E-04

 new geometry:
                                angstroms
 atom            x                  y                  z
 H1       -1.1869213278      1.8851642057     -2.2315701173
 C1       -1.1027279182      2.1186134627     -1.1838049741
 C2       -0.8799920433      2.6952093238      1.5026975236
 C3       -0.8819477140      1.0852623750     -0.2885924909
 C4       -1.2066245591      3.4334659187     -0.7606667434
 C5       -1.0949282193      3.7136871647      0.5886801542
 C6       -0.7684297722      1.3764467780      1.0728913710
 C7       -0.7886740858     -0.3540376693     -0.7559771835
 H3       -1.3740407952      4.2215403347     -1.4725119437
 H4       -1.1787019470      4.7264415871      0.9416033786
 H6       -0.8061475133      2.9353203553      2.5453716288
 C16       0.6117494741     -0.7639232359     -1.2101429052
 C8       -1.3975964479     -1.2513757799      0.3440556445
 N2       -0.5129988503      0.3371915589      1.9945382364
 C9       -0.7759583656     -0.9789520644      1.7035240353
 C10       0.0022451046      0.6567348640      3.3182729298
 O1       -0.5636665830     -1.8545470814      2.4937709467
 C23      -1.3903532666     -2.7427478752      0.0245911186
 C18       3.1403394605     -1.5795030701     -2.0938031075
 C19       0.7610110689     -1.4804890283     -2.3926217082
 C20       1.7572148973     -0.4523576607     -0.4816089039
 C21       3.0070776143     -0.8591712688     -0.9168016007
 C22       2.0112503391     -1.8867327829     -2.8330090636
 H2       -0.1086894815     -1.7262497063     -2.9781239639
 H5        1.6801353578      0.1170682203      0.4257018532
 H7        3.8779579989     -0.6094026362     -0.3365260530
 H8        2.0995345144     -2.4401718887     -3.7516935852
 H9        4.1126448744     -1.8926655170     -2.4311591531
 H10      -1.4353084823     -0.4561214569     -1.6210575160
 H19      -0.3818935893     -3.1312719704     -0.0205739621
 H20      -1.8709488458     -2.9200083396     -0.9329234580
 H21      -1.9245227348     -3.2933123078      0.7864924764
 H22      -2.4332857294     -0.9256232441      0.4454902988
 H11       0.8276287165      1.3539058026      3.2331626783
 H12       0.3447554438     -0.2557767715      3.7741173115
 H13      -0.7658878004      1.0943335119      3.9487948269

 nuclear repulsion energy.......  1415.115717936 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  19   /
------------------------------------------------

 end of program geopt


 start of program onee
```

```
  smallest eigenvalue of S:    3.332E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    324
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
147
  grid # 4      224    223    207    342    311    387    293
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      256    144    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
```

```
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    223    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3728
  grid # 3      214    215    212    215   7185
  grid # 4      211    213    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03319009415           1.5E-05  6.1E-04
etot   2  Y  Y  4  M  -783.03322418596  3.4E-05  6.1E-06  1.5E-04
etot   3  Y  Y  4  M  -783.03322720334  3.0E-06  1.8E-06  2.8E-05
etot   4  Y  N  4  M  -783.03322677979 -4.2E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.11571793578
   (E)  Total one-electron terms..... -3874.79934611265
   (I)  Total two-electron terms.....  1676.65040139707
   (L)  Electronic energy............. -2198.14894471557  (E+I)
   (N)  Total energy.................  -783.03322677979  (A+L)

 SCFE: SCF energy: HF    -783.03322677979 hartrees   iterations:
4


 HOMO energy:    -0.30198
 LUMO energy:     0.12920

  Orbital energies:
  -20.52689  -15.60043  -11.34603  -11.28604  -11.25662  -11.24992
  -11.24287  -11.24152  -11.24053  -11.23854  -11.23787  -11.23490
  -11.23123  -11.23053  -11.22998  -11.22956  -11.22854  -11.22771
```

```
 -11.20890   -1.39766   -1.26976   -1.16510   -1.14895   -1.10610
  -1.03009   -1.01860   -1.01784   -1.01273   -0.96264   -0.93277
  -0.85821   -0.83902   -0.83326   -0.82165   -0.79611   -0.74118
  -0.71111   -0.69496   -0.67302   -0.66427   -0.64455   -0.63767
  -0.62742   -0.61480   -0.61224   -0.60865   -0.59707   -0.58335
  -0.57632   -0.55313   -0.54878   -0.54064   -0.53122   -0.51904
  -0.51497   -0.50725   -0.50097   -0.49782   -0.48461   -0.46863
  -0.46287   -0.42170   -0.41155   -0.34256   -0.33295   -0.32285
  -0.30198    0.12920    0.13404    0.14457    0.15239    0.20403
   0.22972    0.24104    0.24841    0.26131    0.28775

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.995924E-05	4.185434E-05	-2.873563E-05
2	C1	-1.960180E-07	1.077561E-04	1.067132E-05
3	C2	-8.150943E-05	-3.242880E-05	-4.345317E-05
4	C3	7.229837E-05	7.651135E-05	2.084989E-05
5	C4	-1.862976E-05	-7.091458E-05	-1.045063E-04
6	C5	2.811043E-05	-3.749627E-05	5.588205E-05
7	C6	-1.185317E-04	2.924897E-04	-1.619956E-04
8	C7	-3.449398E-05	9.940737E-05	3.539759E-05
9	H3	-1.410742E-05	4.833181E-05	-4.112592E-05
10	H4	2.501973E-07	6.034994E-05	-1.837358E-05
11	H6	-4.285278E-05	1.021627E-05	-7.868038E-06
12	C16	-8.794237E-05	5.999670E-05	8.662938E-05
13	C8	2.056924E-04	1.189359E-06	-2.112645E-04
14	N2	2.207783E-04	4.993886E-04	5.708548E-04
15	C9	-1.993055E-04	1.450186E-05	-4.086489E-04
16	C10	-2.213764E-05	6.483699E-05	1.167574E-04
17	O1	-5.757380E-05	-3.142234E-04	4.001261E-04
18	C23	-1.362736E-04	1.945993E-04	-1.291335E-05
19	C18	1.119864E-04	9.333826E-06	-2.841677E-06
20	C19	-2.675892E-04	5.800909E-05	9.349949E-06
21	C20	-2.130868E-04	1.848689E-05	-1.272899E-04
22	C21	-5.330305E-05	4.347167E-06	-3.964864E-05
23	C22	1.056804E-04	-8.952965E-05	-1.436730E-04
24	H2	-2.627681E-05	3.768385E-05	2.389065E-05

```
  25    H5      5.199311E-06   5.874129E-05   5.445997E-05
  26    H7      9.213307E-05   4.812559E-05   3.019152E-05
  27    H8     -3.377849E-06   3.777330E-05   1.108091E-05
  28    H9      3.767726E-05   3.031445E-05  -2.763578E-05
  29    H10    -4.019614E-05   9.783301E-06  -5.311167E-05
  30    H19     3.854815E-04  -1.579547E-04  -1.218912E-04
  31    H20    -3.458420E-05   6.576202E-05  -8.903255E-05
  32    H21    -2.099997E-04  -1.443898E-04   2.280957E-04
  33    H22    -3.277827E-04   7.122900E-05   1.309177E-05
  34    H11    -3.075156E-04  -6.448305E-05  -3.723384E-05
  35    H12     1.659735E-04   6.175396E-05  -1.733431E-05
  36    H13     1.424084E-04  -1.248751E-04  -2.296081E-04
 -----------   -------------  -------------  -------------
    total      -7.435557E-04   1.046478E-03  -2.608565E-04

  end of program der1b


  start of program geopt  20

  geometry optimization step 20
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0209737
   Cos(theta):   0.5437530

   Final level shift:  -1.4188355E-02

  energy change:          -1.1844E-05 *  (  5.0000E-05 )
  gradient maximum:        6.1036E-04 .  (  4.5000E-04 )
  gradient rms:            1.4279E-04 *  (  3.0000E-04 )
  step size:   0.02097  trust radius:   0.02000
  displacement maximum:    1.5788E-02 .  (  1.8000E-03 )
  displacement rms:        1.8989E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.2114E-05    geom step:   2.0974E-
02    full step:   2.0974E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.1281E-03     y:    -2.4002E-04     z:     9.5604E-04

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1833053714      1.8853359354     -2.2320908616
  C1       -1.1002451245      2.1186038392     -1.1842007806
  C2       -0.8806395561      2.6944182754      1.5028696394
```

```
 C3       -0.8814094028      1.0852102029     -0.2887724259
 C4       -1.2033969688      3.4332141773     -0.7608399732
 C5       -1.0933025831      3.7130999140      0.5888506714
 C6       -0.7692064579      1.3761666927      1.0727752446
 C7       -0.7885303740     -0.3542123823     -0.7559696691
 H3       -1.3687995161      4.2216677280     -1.4726399230
 H4       -1.1765899331      4.7258264500      0.9418676882
 H6       -0.8079471835      2.9336123517      2.5458787424
 C16       0.6119695228     -0.7642594387     -1.2096507464
 C8       -1.3991089279     -1.2514934819      0.3431994191
 N2       -0.5135214985      0.3371892012      1.9949943328
 C9       -0.7805610045     -0.9792202208      1.7041286556
 C10       0.0086257308      0.6574337028      3.3144864504
 O1       -0.5746061124     -1.8551559317      2.4962158034
 C23      -1.3897218408     -2.7431351703      0.0243339312
 C18       3.1417846626     -1.5779202565     -2.0934861880
 C19       0.7617907778     -1.4806520936     -2.3919667078
 C20       1.7571264433     -0.4525065239     -0.4813272079
 C21       3.0074909246     -0.8580109015     -0.9166725136
 C22       2.0128058928     -1.8861931965     -2.8322764514
 H2       -0.1077428260     -1.7267331122     -2.9774866665
 H5        1.6798830061      0.1165589631      0.4261079871
 H7        3.8784031526     -0.6070299890     -0.3366478339
 H8        2.1014777661     -2.4396677154     -3.7505383183
 H9        4.1146731703     -1.8896637147     -2.4307648745
 H10      -1.4346917528     -0.4556626616     -1.6216757860
 H19      -0.3803257064     -3.1324814069     -0.0158816632
 H20      -1.8645753190     -2.9198672385     -0.9361571668
 H21      -1.9283396068     -3.2936872082      0.7840256209
 H22      -2.4354182674     -0.9261759581      0.4424027505
 H11       0.8253544502      1.3634347372      3.2235821973
 H12       0.3650207318     -0.2524504530      3.7649874903
 H13      -0.7605808509      1.0849234282      3.9507142535

 nuclear repulsion energy.......  1415.105494706 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  20   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.331E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    207    342    311    387    294
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     81     97     95     96     97     96
112
  grid # 3      256    146    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    222    223    224    203    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
```

```
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3729
  grid # 3      214    214    213    215   7184
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03313287242           2.3E-05  6.6E-04
etot   2  Y  Y  4  M  -783.03321899828  8.6E-05  1.0E-05  1.9E-04
etot   3  Y  Y  4  M  -783.03323067487  1.2E-05  2.8E-06  4.0E-05
etot   4  Y  N  4  M  -783.03322973681 -9.4E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.10549470597
   (E)  Total one-electron terms..... -3874.77941502785
   (I)  Total two-electron terms.....  1676.64069058507
   (L)  Electronic energy............. -2198.13872444278  (E+I)
   (N)  Total energy.................  -783.03322973681  (A+L)

 SCFE: SCF energy: HF    -783.03322973681 hartrees   iterations:
4


 HOMO energy:    -0.30199
 LUMO energy:     0.12925

  Orbital energies:
  -20.52702  -15.60029  -11.34620  -11.28576  -11.25654  -11.24988
  -11.24300  -11.24141  -11.24041  -11.23858  -11.23785  -11.23474
  -11.23139  -11.23050  -11.23007  -11.22972  -11.22857  -11.22756
  -11.20918   -1.39736   -1.26971   -1.16514   -1.14901   -1.10611
   -1.03010   -1.01866   -1.01793   -1.01267   -0.96263   -0.93271
   -0.85813   -0.83889   -0.83332   -0.82168   -0.79610   -0.74112
   -0.71108   -0.69501   -0.67296   -0.66430   -0.64453   -0.63770
   -0.62741   -0.61486   -0.61227   -0.60869   -0.59718   -0.58328
   -0.57637   -0.55332   -0.54871   -0.54056   -0.53111   -0.51900
   -0.51496   -0.50724   -0.50100   -0.49783   -0.48461   -0.46860
   -0.46289   -0.42156   -0.41155   -0.34262   -0.33290   -0.32296
   -0.30199    0.12925    0.13407    0.14450    0.15241    0.20384
```

```
   0.22965    0.24101    0.24838    0.26132    0.28771

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.009584E-05	4.453890E-05	-1.656705E-05
2	C1	-3.624155E-05	9.076605E-05	-6.143301E-05
3	C2	-8.332459E-05	2.118353E-04	8.658905E-05
4	C3	5.878813E-05	-1.941010E-04	5.590234E-05
5	C4	-7.830940E-06	1.409806E-04	8.425844E-05
6	C5	-4.583976E-05	1.319556E-04	-1.483254E-04
7	C6	1.305104E-04	-7.464085E-05	-8.405979E-05
8	C7	-1.444378E-04	1.465998E-04	-8.993895E-05
9	H3	-4.698580E-05	6.615517E-05	-5.238163E-05
10	H4	-1.983840E-05	7.168568E-05	-3.528920E-05
11	H6	-8.840291E-05	7.624076E-05	-3.467215E-05
12	C16	-2.403805E-04	-1.981480E-05	3.934235E-06
13	C8	2.622219E-04	6.777909E-05	-1.128201E-04
14	N2	-6.148925E-05	-6.644672E-04	-1.072586E-03
15	C9	-1.204331E-04	2.860748E-04	5.164296E-04
16	C10	-4.050302E-04	-1.035969E-04	4.806264E-04
17	O1	1.482384E-04	5.325488E-04	6.573544E-06
18	C23	1.203653E-04	-1.556499E-04	1.144266E-04
19	C18	4.959999E-05	-7.410238E-05	-1.218329E-04
20	C19	1.769771E-04	-1.301900E-04	-2.283536E-04
21	C20	1.379351E-04	1.162175E-04	5.316206E-05
22	C21	6.991646E-05	1.877272E-04	2.528542E-04
23	C22	-3.325628E-04	6.166054E-05	-8.932275E-07
24	H2	4.711591E-06	1.411501E-05	-1.467632E-05
25	H5	-1.410939E-05	1.194850E-04	1.326006E-04
26	H7	-4.237038E-05	1.177471E-05	3.532720E-05
27	H8	-1.636822E-05	-4.542926E-05	-1.777285E-04
28	H9	-6.929392E-05	6.581016E-06	-3.022013E-05
29	H10	3.661675E-05	-3.057423E-06	3.306135E-05
30	H19	-2.384512E-04	1.871304E-04	-3.286634E-05
31	H20	-1.271449E-04	-4.121440E-05	7.115128E-06
32	H21	4.262770E-05	6.082022E-05	-1.799689E-04
33	H22	-1.572623E-04	-3.964235E-05	-1.049391E-05

```
 34    H11    -1.477178E-04   6.129591E-05   1.481875E-04
 35    H12     3.914222E-05  -1.903404E-05   1.183709E-04
 36    H13     4.688385E-04  -8.952801E-05   1.368794E-04
-----------   -------------  -------------  -------------
   total      -7.191221E-04   1.039499E-03  -2.388085E-04

 end of program der1b


 start of program geopt  21

 geometry optimization step 21
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0106758
  Cos(theta):   0.6455990

  Final level shift:  -5.5765491E-02

 energy change:          -2.9570E-06 *  (  5.0000E-05 )
 gradient maximum:        1.5133E-03 .  (  4.5000E-04 )
 gradient rms:            2.7032E-04 *  (  3.0000E-04 )
 step size:   0.01068  trust radius:   0.01000
 displacement maximum:    5.5502E-03 .  (  1.8000E-03 )
 displacement rms:        9.6654E-04 *  (  1.2000E-03 )
 predicted energy change:    -1.3467E-05    geom step:   1.0676E-
02    full step:   1.0676E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:     1.6099E-03     y:     6.5865E-04     z:    -7.4481E-04

 new geometry:
                                angstroms
 atom            x                 y                 z
 H1       -1.1838446186      1.8857210295     -2.2319614009
 C1       -1.1004137980      2.1191013413     -1.1841237428
 C2       -0.8809630112      2.6956465123      1.5026239201
 C3       -0.8802564599      1.0856569582     -0.2887947676
 C4       -1.2047158991      3.4339750976     -0.7611045440
 C5       -1.0949839810      3.7141515292      0.5883840002
 C6       -0.7675108398      1.3770076252      1.0726458703
 C7       -0.7879093639     -0.3538148843     -0.7558731683
 H3       -1.3714121764      4.2220009569     -1.4731876393
 H4       -1.1797176634      4.7268669894      0.9411683427
 H6       -0.8094456879      2.9353014578      2.5455772599
 C16       0.6120687758     -0.7645848589     -1.2105252148
```

```
  C8       -1.3971522040     -1.2513055534      0.3440516203
  N2       -0.5119723496      0.3376603575      1.9941243738
  C9       -0.7783788699     -0.9778680155      1.7047852932
  C10       0.0023010936      0.6558796803      3.3188522462
  O1       -0.5702014687     -1.8522892703      2.4974584523
  C23      -1.3882508626     -2.7429017787      0.0251984336
  C18       3.1399991444     -1.5808736028     -2.0951812321
  C19       0.7606934712     -1.4809832169     -2.3931859698
  C20       1.7578993010     -0.4535446674     -0.4822447350
  C21       3.0074611356     -0.8607324919     -0.9179124878
  C22       2.0105590528     -1.8875816218     -2.8340808691
  H2       -0.1092753969     -1.7262003731     -2.9783532095
  H5        1.6813326902      0.1158099975      0.4253166947
  H7        3.8786604084     -0.6114370400     -0.3378833514
  H8        2.0983840058     -2.4408226043     -3.7528994158
  H9        4.1120590457     -1.8942171409     -2.4330244873
  H10      -1.4347092663     -0.4556836761     -1.6207938681
  H19      -0.3793209703     -3.1303470850     -0.0200773983
  H20      -1.8686925338     -2.9209373142     -0.9322670811
  H21      -1.9219907589     -3.2938616502      0.7871224693
  H22      -2.4335850215     -0.9267821849      0.4437870141
  H11       0.8180908164      1.3640913483      3.2354692278
  H12       0.3576225510     -0.2545222203      3.7694100624
  H13      -0.7692566277      1.0803893955      3.9540632924

  nuclear repulsion energy.......  1415.007074684 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  21   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.333E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
```

```
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
145
  grid # 4      224    223    207    342    311    387    293
277

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     81     97     95     96     97     96
112
  grid # 3      256    148    183    183    182    184    183
212
  grid # 4      450    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    217
217
  grid # 4      207    223    224    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3730
  grid # 3      214    215    213    217   7189
  grid # 4      211    211    209    218   9914

  end of program grid


  start of program rwr
```

```
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                        RMS     maximum
      e  d  i  u  i                        energy  density   DIIS
      r  t  s  t  d     total energy       change  change    error

etot  1  N  N  1  U  -783.03319507055                1.5E-05  5.4E-04
etot  2  Y  Y  4  M  -783.03323060849  3.6E-05  6.3E-06  1.5E-04
etot  3  Y  Y  4  M  -783.03323206347  1.5E-06  2.2E-06  3.3E-05
etot  4  Y  N  4  M  -783.03323263437  5.7E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1415.00707468425
   (E)  Total one-electron terms..... -3874.58115429391
   (I)  Total two-electron terms.....  1676.54084697530
   (L)  Electronic energy............. -2198.04030731862  (E+I)
   (N)  Total energy.................  -783.03323263437  (A+L)

 SCFE: SCF energy: HF    -783.03323263437 hartrees   iterations:
4


 HOMO energy:    -0.30202
 LUMO energy:     0.12920

  Orbital energies:
  -20.52675  -15.60050  -11.34602  -11.28611  -11.25663  -11.24998
  -11.24297  -11.24158  -11.24057  -11.23855  -11.23789  -11.23493
  -11.23121  -11.23054  -11.22998  -11.22957  -11.22852  -11.22773
  -11.20896   -1.39765   -1.26973   -1.16510   -1.14896   -1.10607
   -1.03011   -1.01862   -1.01785   -1.01275   -0.96262   -0.93278
   -0.85823   -0.83906   -0.83328   -0.82167   -0.79612   -0.74120
   -0.71108   -0.69498   -0.67297   -0.66428   -0.64459   -0.63762
   -0.62744   -0.61484   -0.61225   -0.60857   -0.59698   -0.58337
   -0.57631   -0.55323   -0.54884   -0.54065   -0.53114   -0.51906
   -0.51493   -0.50725   -0.50101   -0.49779   -0.48459   -0.46867
   -0.46287   -0.42169   -0.41155   -0.34257   -0.33297   -0.32284
   -0.30202    0.12920    0.13402    0.14456    0.15236    0.20400
    0.22973    0.24104    0.24864    0.26129    0.28791

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.891526E-05	3.681911E-05	-3.883671E-05
2	C1	4.098733E-06	8.305300E-05	-1.179986E-05
3	C2	-4.127792E-05	-1.217594E-04	-9.203155E-05
4	C3	1.449174E-05	1.103326E-04	2.951615E-05
5	C4	-2.717421E-05	-1.235957E-04	-1.460539E-04
6	C5	3.683159E-05	-3.925613E-05	1.270241E-04
7	C6	-1.859365E-04	3.429035E-04	-1.042361E-04
8	C7	4.684163E-05	-8.246545E-06	5.775395E-05
9	H3	-1.136830E-05	5.158783E-05	-3.886596E-05
10	H4	-6.403389E-06	6.688649E-05	7.237490E-07
11	H6	-3.100028E-05	1.744437E-05	2.001002E-05
12	C16	7.212567E-06	1.238818E-04	1.294888E-04
13	C8	2.441704E-05	5.198429E-05	-1.180939E-04
14	N2	2.533677E-04	5.402540E-04	8.460801E-04
15	C9	-9.207294E-05	-5.251305E-05	-5.716448E-04
16	C10	-3.615908E-05	1.775448E-04	5.722617E-05
17	O1	-1.332531E-04	-4.237311E-04	3.247466E-04
18	C23	-1.433637E-04	2.234657E-04	-7.140343E-05
19	C18	1.164926E-04	3.011888E-05	2.193885E-05
20	C19	-3.090097E-04	1.136871E-04	7.854669E-05
21	C20	-2.488769E-04	4.906342E-05	-6.082866E-05
22	C21	-5.325715E-05	-2.207554E-05	-7.465116E-05
23	C22	1.710025E-04	-8.526338E-05	-1.280411E-04
24	H2	-7.478480E-05	1.927847E-05	-2.146933E-05
25	H5	-2.973703E-06	-3.230521E-06	-3.046197E-05
26	H7	8.801257E-05	4.441310E-05	2.493007E-05
27	H8	-2.565978E-06	2.832492E-05	-9.470991E-06
28	H9	5.904517E-05	1.951386E-05	-2.788960E-05
29	H10	-7.270369E-05	2.412400E-05	-7.886933E-05
30	H19	3.535550E-04	-1.588965E-04	-9.565487E-05
31	H20	-6.018620E-06	6.586207E-05	-9.145644E-05
32	H21	-1.860283E-04	-1.213773E-04	2.358173E-04
33	H22	-2.184872E-04	5.954641E-05	2.359554E-05
34	H11	-1.730578E-04	-8.638448E-05	-8.805156E-05
35	H12	1.236212E-04	1.050370E-04	-1.256865E-04
36	H13	2.622021E-05	-8.681337E-05	-2.278204E-04
total		-7.494783E-04	1.051984E-03	-2.759200E-04

```
 end of program der1b
```

```
  start of program geopt  22

  geometry optimization step 22
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0101821
   Cos(theta):   0.7075336

   Final level shift:  -5.2647640E-02

  energy change:          -2.8976E-06 *  (  5.0000E-05 )
  gradient maximum:        7.2565E-04 .  (  4.5000E-04 )
  gradient rms:            1.5949E-04 *  (  3.0000E-04 )
  step size:   0.01018  trust radius:   0.01000
  displacement maximum:    6.2505E-03 .  (  1.8000E-03 )
  displacement rms:        9.2184E-04 *  (  1.2000E-03 )
  predicted energy change:    -9.0748E-06    geom step:   1.0182E-
02    full step:   1.0182E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.3929E-03     y:    -2.8193E-04     z:     6.9961E-04

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1819150396     1.8853922550    -2.2323270409
  C1       -1.0992989228     2.1187762076    -1.1844060309
  C2       -0.8815820860     2.6950766907     1.5027188160
  C3       -0.8806626123     1.0854731666    -0.2886848442
  C4       -1.2028950183     3.4334766868    -0.7614131651
  C5       -1.0939437286     3.7136083695     0.5883486982
  C6       -0.7688426034     1.3767839590     1.0728254098
  C7       -0.7880471035    -0.3540376930    -0.7557727134
  H3       -1.3681439538     4.2217396413    -1.4735567144
  H4       -1.1780020057     4.7264297293     0.9410291195
  H6       -0.8105475239     2.9343387731     2.5458451578
  C16       0.6121509266    -0.7644500039    -1.2099567201
  C8       -1.3984320302    -1.2513737008     0.3435064911
  N2       -0.5125884590     0.3376215864     1.9949682824
  C9       -0.7805205459    -0.9784903779     1.7047948851
  C10       0.0068779638     0.6569622363     3.3162775632
  O1       -0.5757157312    -1.8536596101     2.4980356622
  C23      -1.3884931302    -2.7431703510     0.0246625620
  C18       3.1412984651    -1.5794441393    -2.0946602431
  C19       0.7612996966    -1.4804949526    -2.3927325686
  C20       1.7576783737    -0.4535735564    -0.4816542029
```

```
  C21       3.0077418962     -0.8598857754     -0.9173277593
  C22       2.0119309545     -1.8865869491     -2.8335742306
  H2       -0.1085073890     -1.7258975192     -2.9782114803
  H5        1.6810112496      0.1149985720      0.4261636982
  H7        3.8789075311     -0.6099995691     -0.3371557358
  H8        2.1001468786     -2.4394912529     -3.7523637895
  H9        4.1138566484     -1.8918002132     -2.4323487958
  H10      -1.4344082104     -0.4555899869     -1.6212999706
  H19      -0.3789138206     -3.1316121882     -0.0177324693
  H20      -1.8653528998     -2.9205324456     -0.9347511236
  H21      -1.9251914574     -3.2941968030      0.7853139446
  H22      -2.4352334309     -0.9269095552      0.4425019773
  H11       0.8195433734      1.3677845721      3.2278540324
  H12       0.3686498275     -0.2520725686      3.7642217714
  H13      -0.7641492419      1.0781467248      3.9540976663

  nuclear repulsion energy.......  1414.981356114 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  22   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.332E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
```

```
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    207    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      256    145    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3728
  grid # 3      214    214    213    217   7185
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
```

```
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -783.03320706613           1.4E-05  3.7E-04
etot   2  Y  Y  4  M  -783.03323229466  2.5E-05  5.5E-06  9.8E-05
etot   3  Y  Y  4  M  -783.03323618442  3.9E-06  1.8E-06  2.7E-05
etot   4  Y  N  4  M  -783.03323580747 -3.8E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.98135611356
   (E)  Total one-electron terms..... -3874.53252926674
   (I)  Total two-electron terms.....  1676.51793734571
   (L)  Electronic energy............. -2198.01459192103  (E+I)
   (N)  Total energy.................  -783.03323580747  (A+L)

 SCFE: SCF energy: HF    -783.03323580747 hartrees   iterations:
4


 HOMO energy:    -0.30201
 LUMO energy:     0.12923

  Orbital energies:
  -20.52695  -15.60031  -11.34612  -11.28586  -11.25655  -11.24990
  -11.24304  -11.24145  -11.24046  -11.23861  -11.23788  -11.23483
  -11.23138  -11.23057  -11.23008  -11.22972  -11.22861  -11.22762
  -11.20916   -1.39734   -1.26958   -1.16510   -1.14898   -1.10605
   -1.03006   -1.01866   -1.01789   -1.01267   -0.96259   -0.93269
   -0.85812   -0.83889   -0.83330   -0.82168   -0.79608   -0.74110
   -0.71102   -0.69499   -0.67291   -0.66427   -0.64454   -0.63764
   -0.62741   -0.61486   -0.61226   -0.60861   -0.59708   -0.58329
   -0.57634   -0.55331   -0.54872   -0.54060   -0.53107   -0.51899
   -0.51493   -0.50721   -0.50099   -0.49780   -0.48460   -0.46860
   -0.46287   -0.42156   -0.41154   -0.34261   -0.33290   -0.32293
   -0.30201    0.12923    0.13405    0.14450    0.15238    0.20384
    0.22969    0.24101    0.24855    0.26131    0.28781

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.916563E-05	3.115840E-05	-2.179536E-06
2	C1	-3.176839E-05	5.571029E-05	-4.887123E-05
3	C2	-8.364972E-05	1.522264E-04	5.976368E-05
4	C3	5.657305E-05	-1.107126E-04	3.655009E-06
5	C4	-1.432425E-05	1.292198E-04	8.364702E-05
6	C5	-4.711387E-05	9.593937E-05	-1.181324E-04
7	C6	1.462065E-04	-1.417284E-04	-1.954080E-05
8	C7	-1.447753E-04	1.209384E-04	-5.869440E-05
9	H3	-3.303763E-05	4.074427E-05	-1.765869E-05
10	H4	-2.422724E-05	3.672910E-05	-2.063647E-05
11	H6	-5.377233E-05	5.986436E-05	-2.376962E-05
12	C16	-1.437880E-04	-3.278992E-05	-2.384321E-05
13	C8	1.682461E-04	-8.141492E-06	-6.768585E-05
14	N2	-8.685477E-05	-3.125792E-04	-7.054728E-04
15	C9	-1.669181E-04	1.614411E-04	3.996291E-04
16	C10	-1.705983E-04	-6.270829E-05	1.695849E-04
17	O1	7.917364E-05	3.825163E-04	-6.811426E-05
18	C23	7.817251E-05	-9.317944E-05	1.096917E-04
19	C18	-2.707985E-05	-1.515457E-05	-5.897308E-05
20	C19	1.350316E-04	-7.162433E-05	-1.525613E-04
21	C20	1.302495E-04	3.667741E-05	-9.903622E-06
22	C21	1.332486E-05	1.051566E-04	1.162654E-04
23	C22	-2.098854E-04	8.554273E-05	4.232424E-05
24	H2	1.018806E-05	3.065519E-05	1.245542E-05
25	H5	-3.460981E-05	1.179006E-04	1.076225E-04
26	H7	-5.668086E-05	1.274230E-05	2.399314E-06
27	H8	-2.503916E-05	-1.818965E-05	-9.525772E-05
28	H9	-6.442969E-05	1.802301E-05	-1.209761E-05
29	H10	1.346558E-05	2.416650E-05	2.960450E-05
30	H19	-1.897929E-04	1.508450E-04	-1.976906E-05
31	H20	-8.748547E-05	1.919435E-06	-2.239334E-06
32	H21	4.575604E-05	7.082458E-05	-1.291513E-04
33	H22	-2.398281E-05	-1.698642E-05	-1.164509E-05
34	H11	-1.125323E-04	7.734529E-05	8.992237E-05
35	H12	1.381562E-05	-2.480412E-05	7.722300E-05
36	H13	2.164018E-04	-3.414594E-05	1.084480E-04
total		-7.449070E-04	1.055542E-03	-2.539613E-04

```
 end of program der1b


 start of program geopt  23

 geometry optimization step 23
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
```

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0104114
   Cos(theta):   0.5769708

   Final level shift:  -2.1612403E-02

  energy change:          -3.1731E-06 *  (  5.0000E-05 )
  gradient maximum:        8.7985E-04 .  (  4.5000E-04 )
  gradient rms:            1.6127E-04 *  (  3.0000E-04 )
  step size:   0.01041  trust radius:   0.01000
  displacement maximum:    5.3754E-03 .  (  1.8000E-03 )
  displacement rms:        9.4260E-04 *  (  1.2000E-03 )
  predicted energy change:    -6.5215E-06    geom step:   1.0411E-
02    full step:   1.0411E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.2579E-03     y:     4.7140E-04     z:    -6.3420E-04

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1816446534     1.8860188338    -2.2320885598
  C1       -1.0988308566     2.1194141523    -1.1842049520
  C2       -0.8815693026     2.6959102616     1.5027623991
  C3       -0.8793851855     1.0859276017    -0.2887051317
  C4       -1.2033638261     3.4342905921    -0.7612244278
  C5       -1.0948884741     3.7144464052     0.5884118539
  C6       -0.7672586342     1.3773786532     1.0727619828
  C7       -0.7875246295    -0.3535936423    -0.7556999900
  H3       -1.3694746100     4.2223385591    -1.4734216231
  H4       -1.1801742422     4.7271379584     0.9411857885
  H6       -0.8116216846     2.9354342423     2.5458768303
  C16       0.6121905304    -0.7647189853    -1.2108474660
  C8       -1.3965841893    -1.2512669058     0.3441333065
  N2       -0.5113647159     0.3380794758     1.9940939242
  C9       -0.7791067321    -0.9773815422     1.7054060916
  C10       0.0007927325     0.6560275462     3.3198175565
  O1       -0.5731796269    -1.8514631705     2.4991142258
  C23      -1.3863602017    -2.7428795023     0.0254239622
  C18       3.1395358234    -1.5822072954    -2.0962180229
  C19       0.7601458020    -1.4811979517    -2.3935737757
  C20       1.7583763239    -0.4539639278    -0.4830123904
  C21       3.0076112244    -0.8619491044    -0.9189251455
  C22       2.0097727254    -1.8882992039    -2.8348984867
  H2       -0.1101211313    -1.7261351586    -2.9783475197
  H5        1.6822379420     0.1157928183     0.4244442004
  H7        3.8790653710    -0.6131773248    -0.3390483679
  H8        2.0971294650    -2.4414102478    -3.7538805512
  H9        4.1113598146    -1.8960676301    -2.4343044753
  H10      -1.4345549296    -0.4552095349    -1.6204796491
```

```
  H19      -0.3771008992     -3.1286638251     -0.0229127545
  H20      -1.8691322668     -2.9218045999     -0.9306772532
  H21      -1.9170387269     -3.2945279056      0.7888262681
  H22      -2.4333412917     -0.9277555858      0.4433950528
  H11       0.8120194967      1.3694773054      3.2379328771
  H12       0.3622400391     -0.2533320682      3.7675391697
  H13      -0.7731139506      1.0736904080      3.9566629542

  nuclear repulsion energy.......  1414.949804110 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  23   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.334E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
145
  grid # 4      224    223    207    342    311    387    293
276
```

```
  number of gridpoints:
     atom         O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1       111     73     89     88     88     89     89
71
  grid # 2       123     80     97     95     96     97     96
112
  grid # 3       256    147    183    183    182    184    183
212
  grid # 4       450    286    327    326    327    327    327
211

  number of gridpoints:
     atom         H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1        71     73     73     73     66     71     71
70
  grid # 2       111    118    118    118    106    108    110
108
  grid # 3       212    223    223    224    202    218    217
217
  grid # 4       207    223    224    224    197    212    216
215

  number of gridpoints:
     atom        H22    H11    H12    H13  total
  grid # 1        69     71     70     71   2862
  grid # 2       110    109    107    111   3729
  grid # 3       214    215    213    217   7188
  grid # 4       211    211    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy       change  change    error

etot   1  N  N  1  U  -783.03321038208                1.4E-05  5.2E-04
etot   2  Y  Y  4  M  -783.03324043608  3.0E-05  5.8E-06  1.4E-04
etot   3  Y  Y  4  M  -783.03324163186  1.2E-06  1.9E-06  2.6E-05
etot   4  Y  N  4  M  -783.03324220777  5.8E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
```

```
   (A)  Nuclear repulsion.....  1414.94980411001
   (E)  Total one-electron terms..... -3874.46676102956
   (I)  Total two-electron terms.....  1676.48371471178
   (L)  Electronic energy..... -2197.98304631778  (E+I)
   (N)  Total energy.............  -783.03324220777  (A+L)

 SCFE: SCF energy: HF    -783.03324220777 hartrees   iterations:
4


 HOMO energy:    -0.30201
 LUMO energy:     0.12922

  Orbital energies:
 -20.52677  -15.60051  -11.34603  -11.28611  -11.25664  -11.24997
 -11.24297  -11.24158  -11.24056  -11.23856  -11.23790  -11.23493
 -11.23124  -11.23053  -11.22999  -11.22957  -11.22854  -11.22774
 -11.20889   -1.39762   -1.26972   -1.16509   -1.14895   -1.10606
  -1.03011   -1.01862   -1.01785   -1.01274   -0.96260   -0.93279
  -0.85824   -0.83906   -0.83328   -0.82167   -0.79611   -0.74121
  -0.71105   -0.69498   -0.67294   -0.66430   -0.64461   -0.63758
  -0.62744   -0.61486   -0.61226   -0.60856   -0.59696   -0.58337
  -0.57631   -0.55327   -0.54885   -0.54070   -0.53111   -0.51905
  -0.51490   -0.50725   -0.50102   -0.49777   -0.48458   -0.46869
  -0.46286   -0.42171   -0.41157   -0.34258   -0.33296   -0.32284
  -0.30201    0.12922    0.13402    0.14455    0.15235    0.20397
   0.22976    0.24106    0.24880    0.26128    0.28806

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1     -2.070945E-05   4.024664E-05  -3.696400E-05
   2    C1     -1.211440E-05   8.045173E-05   1.551131E-05
   3    C2     -5.851773E-05  -9.877886E-05  -6.424861E-05
   4    C3     -7.218233E-06   1.493799E-04   2.489292E-05
   5    C4     -1.864256E-05  -1.193946E-04  -1.297161E-04
   6    C5      1.723854E-05  -4.299501E-05   8.576822E-05
   7    C6     -1.601198E-04   3.097136E-04  -1.518652E-04
```

8	C7	9.039535E-05	-4.495661E-06	2.631682E-05
9	H3	-1.316263E-05	4.992671E-05	-3.764982E-05
10	H4	-1.012040E-05	5.264121E-05	-5.212269E-06
11	H6	-9.797036E-06	9.606623E-06	1.643370E-05
12	C16	1.822479E-05	1.347772E-04	8.770785E-05
13	C8	2.804277E-05	2.761058E-05	-8.357224E-05
14	N2	1.735992E-04	4.445849E-04	9.831983E-04
15	C9	-9.363108E-05	-5.491115E-05	-5.715093E-04
16	C10	4.681529E-05	1.249793E-04	-6.740218E-05
17	O1	-1.078267E-04	-3.223177E-04	2.676191E-04
18	C23	-2.016860E-04	2.788180E-04	-1.415645E-04
19	C18	1.041047E-04	3.690554E-05	2.358251E-05
20	C19	-2.305009E-04	1.160960E-04	9.775743E-05
21	C20	-2.570654E-04	6.235023E-05	-1.054657E-05
22	C21	-5.126104E-05	-1.409648E-05	-7.187286E-05
23	C22	1.198616E-04	-6.656572E-05	-1.202745E-04
24	H2	-9.084589E-05	1.739289E-05	-4.508372E-05
25	H5	8.936467E-06	-5.774461E-05	-7.264259E-05
26	H7	8.927311E-05	4.853633E-05	2.010690E-05
27	H8	-7.709163E-06	3.583026E-05	1.809475E-05
28	H9	5.218324E-05	2.479653E-05	-1.890401E-05
29	H10	-7.345051E-05	2.019126E-05	-7.734345E-05
30	H19	4.623240E-04	-2.116910E-04	-5.541436E-05
31	H20	-9.581257E-06	8.544252E-05	-1.137165E-04
32	H21	-2.332082E-04	-1.470636E-04	2.808667E-04
33	H22	-2.439216E-04	9.240509E-05	2.349342E-05
34	H11	-1.495754E-04	-7.325640E-05	-7.276418E-05
35	H12	1.136216E-04	8.450404E-05	-6.962532E-05
36	H13	-2.038626E-05	-5.169248E-05	-2.480026E-04
total		-7.564309E-04	1.062184E-03	-2.945450E-04

end of program der1b

start of program geopt 24

geometry optimization step 24
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format

Level shifts adjusted to satisfy step-size constraints
Step size: 0.0103362
Cos(theta): 0.7418847

Final level shift: -5.9053150E-02

energy change: -6.4003E-06 * (5.0000E-05)
gradient maximum: 6.3424E-04 . (4.5000E-04)

```
  gradient rms:            1.5766E-04 *  (  3.0000E-04 )
  step size:   0.01034  trust radius:   0.01000
  displacement maximum:    4.7916E-03 .  (  1.8000E-03 )
  displacement rms:        9.3580E-04 *  (  1.2000E-03 )
  predicted energy change:    -9.8314E-06    geom step:   1.0336E-
02    full step:   1.0336E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.3819E-03     y:    -2.5555E-04     z:     6.7702E-04

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1807662982     1.8856546836    -2.2324339186
  C1       -1.0985716874     2.1190663819    -1.1844790358
  C2       -0.8823965292     2.6953781592     1.5027534870
  C3       -0.8800839607     1.0857690408    -0.2886561974
  C4       -1.2026989145     3.4337393358    -0.7615758193
  C5       -1.0946422101     3.7138668991     0.5882588199
  C6       -0.7686879634     1.3771365281     1.0728545222
  C7       -0.7876740786    -0.3537518831    -0.7557479976
  H3       -1.3678671160     4.2219535647    -1.4738317131
  H4       -1.1793917086     4.7266655453     0.9408812366
  H6       -0.8124043991     2.9345532630     2.5459876453
  C16       0.6123021076    -0.7644310328    -1.2102547600
  C8       -1.3980075808    -1.2512844801     0.3434497722
  N2       -0.5118013241     0.3379589468     1.9949245623
  C9       -0.7809287899    -0.9779496153     1.7051040694
  C10       0.0066637971     0.6570697614     3.3167062714
  O1       -0.5774509001    -1.8526661559     2.4992023315
  C23      -1.3869939935    -2.7431586895     0.0248811929
  C18       3.1409487851    -1.5809233104    -2.0950441477
  C19       0.7610481805    -1.4799405014    -2.3934595659
  C20       1.7579703603    -0.4547311572    -0.4816177477
  C21       3.0078053971    -0.8618880144    -0.9172769401
  C22       2.0114262547    -1.8866939350    -2.8344081754
  H2       -0.1089117793    -1.7244399139    -2.9791423755
  H5        1.6815762001     0.1131967911     0.4266286700
  H7        3.8790778544    -0.6131220071    -0.3367885296
  H8        2.0993641944    -2.4391128962    -3.7535821537
  H9        4.1132954654    -1.8939255165    -2.4327621039
  H10      -1.4341937564    -0.4552121303    -1.6211777235
  H19      -0.3769739184    -3.1307475786    -0.0187880168
  H20      -1.8646568895    -2.9209082637    -0.9340950704
  H21      -1.9225416771    -3.2945938238     0.7861813177
  H22      -2.4351583627    -0.9274785072     0.4420193319
  H11       0.8160139954     1.3716652852     3.2291481396
  H12       0.3731739390    -0.2509830623     3.7628598241
  H13      -0.7657941424     1.0734962138     3.9557012265

  nuclear repulsion energy.......  1414.931929768 hartrees
```

```
  ------------------------------------------------
 /  end of geometry optimization iteration  24   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.333E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    207    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      256    149    183    183    182    184    183
212
```

```
  grid # 4      450    288    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3728
  grid # 3      214    214    213    217   7189
  grid # 4      211    211    209    218   9913

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                              RMS    maximum
      t  p  i  c  r                                  energy  density   DIIS
      e  d  i  u  i                 total energy     change  change    error

etot  1  N  N  1  U  -783.03320679670                        1.3E-05  4.3E-04
etot  2  Y  Y  4  M  -783.03323432207  2.8E-05  5.5E-06  1.2E-04
etot  3  Y  Y  4  M  -783.03323964878  5.3E-06  1.8E-06  2.5E-05
etot  4  Y  N  4  M  -783.03323983242  1.8E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.93192976811
   (E)  Total one-electron terms..... -3874.43430858270
   (I)  Total two-electron terms.....  1676.46913898216
   (L)  Electronic energy............. -2197.96516960053  (E+I)
   (N)  Total energy.................  -783.03323983242  (A+L)

 SCFE: SCF energy: HF    -783.03323983242 hartrees   iterations:
4
```

```
HOMO energy:    -0.30202
LUMO energy:     0.12924

 Orbital energies:
 -20.52693  -15.60030  -11.34609  -11.28587  -11.25654  -11.24990
 -11.24308  -11.24145  -11.24047  -11.23863  -11.23788  -11.23485
 -11.23140  -11.23059  -11.23008  -11.22974  -11.22863  -11.22763
 -11.20919   -1.39732   -1.26953   -1.16508   -1.14897   -1.10603
  -1.03004   -1.01865   -1.01788   -1.01267   -0.96258   -0.93268
  -0.85811   -0.83888   -0.83329   -0.82168   -0.79607   -0.74109
  -0.71100   -0.69499   -0.67287   -0.66427   -0.64455   -0.63762
  -0.62742   -0.61487   -0.61226   -0.60859   -0.59705   -0.58329
  -0.57633   -0.55331   -0.54870   -0.54062   -0.53104   -0.51896
  -0.51491   -0.50720   -0.50099   -0.49778   -0.48459   -0.46861
  -0.46287   -0.42154   -0.41153   -0.34261   -0.33291   -0.32292
  -0.30202    0.12924    0.13404    0.14448    0.15237    0.20382
   0.22969    0.24102    0.24863    0.26129    0.28787

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H1     -1.830432E-05   2.859732E-05   1.799449E-06
  2    C1     -4.225191E-05   3.026880E-05  -5.166108E-05
  3    C2     -8.924106E-05   1.426865E-04   4.865788E-05
  4    C3      3.186071E-05  -8.915463E-05  -1.801414E-05
  5    C4     -9.228697E-06   1.322182E-04   7.897200E-05
  6    C5     -4.994730E-05   9.639113E-05  -8.425225E-05
  7    C6      1.909008E-04  -1.367827E-04   2.604393E-05
  8    C7     -1.444191E-04   8.844947E-05  -7.431758E-05
  9    H3     -2.358052E-05   2.762505E-05  -2.190934E-06
 10    H4     -2.299433E-05   2.387232E-05  -1.594406E-05
 11    H6     -4.232650E-05   5.906493E-05  -2.864193E-05
 12    C16    -1.094051E-04  -5.524783E-05  -2.889432E-05
 13    C8      1.601065E-04   2.672291E-05   8.991977E-07
 14    N2     -1.830085E-04  -2.532448E-04  -7.895700E-04
 15    C9     -1.147255E-04   1.488745E-04   4.702422E-04
 16    C10    -5.628888E-05  -7.425619E-05   1.035672E-04
```

```
  17    O1      5.280779E-05   3.317606E-04  -1.093195E-04
  18    C23     9.574981E-05  -1.351086E-04   7.925995E-05
  19    C18    -6.525682E-05   4.204676E-06  -5.620663E-05
  20    C19     1.295488E-04  -5.038010E-05  -1.344954E-04
  21    C20     1.407837E-04  -7.205440E-06  -2.976252E-05
  22    C21    -2.045950E-05   9.271159E-05   6.276487E-05
  23    C22    -1.671824E-04   8.438955E-05   5.867880E-05
  24    H2      2.773290E-05   3.459095E-05   2.461389E-05
  25    H5     -3.896956E-05   1.323024E-04   9.872315E-05
  26    H7     -5.513480E-05   1.895928E-05  -1.355676E-06
  27    H8     -2.681121E-05  -1.571614E-06  -5.494645E-05
  28    H9     -6.626943E-05   2.257754E-05  -7.835577E-06
  29    H10     1.589811E-05   3.510932E-05   3.253099E-05
  30    H19    -2.933243E-04   1.877127E-04   1.761686E-05
  31    H20    -8.227229E-05  -1.239004E-05   1.794728E-05
  32    H21     9.491791E-05   1.067485E-04  -1.875586E-04
  33    H22     3.766051E-05  -3.179320E-05  -1.313377E-05
  34    H11    -1.021985E-04   9.925423E-05   7.489152E-05
  35    H12    -3.562978E-05  -3.779806E-05   6.234155E-05
  36    H13     1.401746E-04   1.704115E-06   1.640490E-04
 -----------   -------------  -------------  -------------
    total      -7.410881E-04   1.071863E-03  -2.645007E-04

  end of program der1b


  start of program geopt  25

  geometry optimization step 25
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0102317
   Cos(theta):   0.6059804

   Final level shift:  -2.3824706E-02

  energy change:           2.3754E-06 #  (  5.0000E-05 )
  gradient maximum:        8.1317E-04 .  (  4.5000E-04 )
  gradient rms:            1.4988E-04 *  (  3.0000E-04 )
  step size:   0.01023  trust radius:   0.01000
  displacement maximum:    5.2594E-03 .  (  1.8000E-03 )
  displacement rms:        9.2634E-04 *  (  1.2000E-03 )
  predicted energy change:    -6.3792E-06    geom step:   1.0232E-
02    full step:   1.0232E-02
  molecular structure not yet converged...

  center of mass moved by:
```

```
   x:     1.2182E-03     y:     3.4642E-04     z:    -5.8767E-04

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1804039999     1.8865506765    -2.2321161448
 C1       -1.0979458841     2.1197950781    -1.1841695308
 C2       -0.8819504447     2.6959285010     1.5030521132
 C3       -0.8788485557     1.0861911235    -0.2887056689
 C4       -1.2026072373     3.4346008623    -0.7610151555
 C5       -1.0948903805     3.7145786646     0.5887517103
 C6       -0.7670907831     1.3775304400     1.0728369744
 C7       -0.7872096931    -0.3533403156    -0.7558015319
 H3       -1.3683433801     4.2227566651    -1.4731740552
 H4       -1.1804898951     4.7272053034     0.9416326705
 H6       -0.8127601577     2.9352172217     2.5462784971
 C16       0.6123887781    -0.7647773781    -1.2109875094
 C8       -1.3964571306    -1.2510942485     0.3438880080
 N2       -0.5110583369     0.3381466621     1.9940124708
 C9       -0.7798538937    -0.9772134846     1.7055811761
 C10       0.0006682762     0.6556728136     3.3199788976
 O1       -0.5755243984    -1.8512285594     2.4998410184
 C23      -1.3859666216    -2.7427352095     0.0250221901
 C18       3.1395517459    -1.5828649472    -2.0964423291
 C19       0.7600496513    -1.4823634202    -2.3930217741
 C20       1.7587733744    -0.4530588405    -0.4839983115
 C21       3.0079124307    -0.8613390850    -0.9199334996
 C22       2.0095783115    -1.8898139852    -2.8343669658
 H2       -0.1103932559    -1.7280220538    -2.9771487571
 H5        1.6828978627     0.1178816238     0.4228049323
 H7        3.8796020456    -0.6117888706    -0.3406665742
 H8        2.0966889948    -2.4438662875    -3.7527428332
 H9        4.1113207918    -1.8969667362    -2.4345012726
 H10      -1.4342215798    -0.4546959930    -1.6206318894
 H19      -0.3765530833    -3.1279792487    -0.0247516341
 H20      -1.8699136387    -2.9218102920    -0.9304891969
 H21      -1.9153998233    -3.2947182580     0.7890333473
 H22      -2.4334141616    -0.9279086722     0.4427811939
 H11       0.8088853669     1.3723792940     3.2387163939
 H12       0.3661605644    -0.2531570552     3.7656532029
 H13      -0.7743209064     1.0689365450     3.9584155598

 nuclear repulsion energy.......  1414.915862762 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  25   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.334E-04
```

```
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    324
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
145
  grid # 4      224    223    207    342    311    387    293
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      256    145    183    183    182    184    183
212
  grid # 4      450    284    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
```

```
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2862
  grid # 2      110    109    107    111   3729
  grid # 3      214    215    213    217   7187
  grid # 4      211    211    209    218   9909

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03320867731             1.5E-05  4.6E-04
etot   2  Y  Y  4  M  -783.03324156469  3.3E-05    6.2E-06  1.5E-04
etot   3  Y  Y  4  M  -783.03324292046  1.4E-06    2.0E-06  4.5E-05
etot   4  Y  N  4  M  -783.03324297419  5.4E-08    0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.91586276151
   (E)  Total one-electron terms..... -3874.39868431811
   (I)  Total two-electron terms.....  1676.44957858241
   (L)  Electronic energy............. -2197.94910573570  (E+I)
   (N)  Total energy.................  -783.03324297419  (A+L)

 SCFE: SCF energy: HF    -783.03324297419 hartrees   iterations:
4


 HOMO energy:    -0.30201
 LUMO energy:     0.12924

  Orbital energies:
  -20.52676  -15.60052  -11.34604  -11.28612  -11.25664  -11.24998
  -11.24299  -11.24159  -11.24055  -11.23856  -11.23791  -11.23493
  -11.23123  -11.23053  -11.22999  -11.22956  -11.22853  -11.22775
```

```
 -11.20889   -1.39759   -1.26972   -1.16510   -1.14896   -1.10605
  -1.03011   -1.01863   -1.01786   -1.01273   -0.96259   -0.93279
  -0.85825   -0.83906   -0.83330   -0.82168   -0.79611   -0.74121
  -0.71104   -0.69499   -0.67292   -0.66430   -0.64462   -0.63756
  -0.62744   -0.61487   -0.61226   -0.60855   -0.59695   -0.58336
  -0.57632   -0.55330   -0.54885   -0.54071   -0.53108   -0.51906
  -0.51487   -0.50724   -0.50104   -0.49776   -0.48458   -0.46869
  -0.46286   -0.42171   -0.41157   -0.34260   -0.33296   -0.32286
  -0.30201    0.12924    0.13403    0.14452    0.15233    0.20396
   0.22978    0.24105    0.24889    0.26127    0.28812

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.968092E-05	4.059452E-05	-3.563156E-05
2	C1	-1.255708E-05	7.480805E-05	3.533041E-05
3	C2	-5.516245E-05	-9.554485E-05	-7.483967E-05
4	C3	-9.093269E-06	1.432046E-04	3.770540E-05
5	C4	-1.865577E-05	-1.090029E-04	-1.124093E-04
6	C5	1.392032E-05	-4.752238E-05	6.120052E-05
7	C6	-1.558093E-04	2.806181E-04	-1.856184E-04
8	C7	9.596427E-05	9.012141E-06	4.135456E-05
9	H3	-1.770964E-05	5.355912E-05	-3.810306E-05
10	H4	-1.481125E-05	5.542708E-05	-6.612463E-06
11	H6	-9.518855E-06	7.658260E-06	2.089616E-05
12	C16	8.574119E-06	1.763392E-04	8.667722E-05
13	C8	-4.729958E-05	4.342477E-06	-8.939448E-05
14	N2	1.368264E-04	3.484693E-04	9.745207E-04
15	C9	-7.617951E-05	-6.249592E-05	-5.650430E-04
16	C10	3.414526E-05	2.479499E-05	-3.665238E-05
17	O1	-9.572887E-05	-2.294846E-04	2.216641E-04
18	C23	-1.836684E-04	2.948296E-04	-1.526026E-04
19	C18	1.263235E-04	4.044260E-05	2.862647E-05
20	C19	-2.016597E-04	8.703282E-05	6.904293E-05
21	C20	-2.180631E-04	1.044137E-04	6.654719E-05
22	C21	-1.275742E-05	1.242325E-06	-1.717270E-05
23	C22	7.379076E-05	-5.504115E-05	-1.213834E-04
24	H2	-1.105447E-04	1.738737E-05	-7.875050E-05

```
 25    H5      1.038653E-05  -1.008110E-04  -9.540420E-05
 26    H7      5.883075E-05   3.648803E-05   1.589415E-05
 27    H8     -1.226783E-05   2.464442E-05  -2.462600E-05
 28    H9      4.165547E-05   2.361456E-05  -1.889777E-05
 29    H10    -7.754345E-05   1.437099E-05  -7.315136E-05
 30    H19     4.502441E-04  -2.163477E-04  -3.872120E-05
 31    H20     5.440984E-06   9.974619E-05  -1.031117E-04
 32    H21    -2.365951E-04  -1.384137E-04   2.866286E-04
 33    H22    -2.064680E-04   1.008538E-04   1.928227E-05
 34    H11    -8.850643E-05  -3.358248E-05  -7.412515E-05
 35    H12     9.804979E-05   1.226769E-04  -5.995003E-05
 36    H13    -2.832963E-05  -3.824437E-05  -2.658042E-04
-----------   -------------  -------------  -------------
   total      -7.544580E-04   1.060080E-03  -3.026344E-04

 end of program der1b


 start of program geopt  26

 geometry optimization step 26
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0108918
  Cos(theta):   0.7490567

  Final level shift:  -6.0844884E-02

 energy change:          -3.1418E-06 *  (  5.0000E-05 )
 gradient maximum:        5.4728E-04 .  (  4.5000E-04 )
 gradient rms:            1.5681E-04 *  (  3.0000E-04 )
 step size:   0.01089  trust radius:   0.01000
 displacement maximum:    4.6624E-03 .  (  1.8000E-03 )
 displacement rms:        9.8610E-04 *  (  1.2000E-03 )
 predicted energy change:    -1.0674E-05    geom step:   1.0892E-
02    full step:   1.0892E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -1.3328E-03     y:    -1.5413E-04     z:     6.1461E-04

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1803188283      1.8858310573     -2.2325079196
 C1       -1.0983798791      2.1192725182     -1.1845309612
 C2       -0.8831564903      2.6956058680      1.5027175681
```

```
 C3       -0.8797272743      1.0860218070     -0.2886596363
 C4       -1.2030303125      3.4339084280     -0.7616847240
 C5       -1.0955651345      3.7140463716      0.5881847040
 C6       -0.7685699692      1.3774337382      1.0727987054
 C7       -0.7873243539     -0.3534566287     -0.7557698634
 H3       -1.3683018364      4.2220668798     -1.4740081869
 H4       -1.1809588303      4.7268113952      0.9407854784
 H6       -0.8138089817      2.9346992945      2.5460376806
 C16       0.6125121393     -0.7642711640     -1.2104786354
 C8       -1.3976264175     -1.2511533629      0.3433646243
 N2       -0.5112137360      0.3382635108      1.9947919352
 C9       -0.7811149874     -0.9774632320      1.7052608228
 C10       0.0069698534      0.6572851155      3.3167423300
 O1       -0.5785186953     -1.8517728847      2.4999897344
 C23      -1.3857702853     -2.7430349910      0.0249957177
 C18       3.1406819904     -1.5823214730     -2.0950829409
 C19       0.7609597083     -1.4791016507     -2.3942363709
 C20       1.7582260179     -0.4561233930     -0.4811421254
 C21       3.0078432614     -0.8641262558     -0.9166963416
 C22       2.0111124135     -1.8864903192     -2.8351648413
 H2       -0.1090809114     -1.7226091469     -2.9803378334
 H5        1.6819419650      0.1107617304      0.4277125316
 H7        3.8791163772     -0.6167474193     -0.3356639889
 H8        2.0988542728     -2.4382308726     -3.7548604062
 H9        4.1128218546     -1.8960089505     -2.4327558471
 H10      -1.4339854287     -0.4548952199     -1.6211161311
 H19      -0.3754689921     -3.1299660689     -0.0192357913
 H20      -1.8637814836     -2.9210961325     -0.9337706651
 H21      -1.9206134298     -3.2947414841      0.7866483229
 H22      -2.4349632292     -0.9278435712      0.4416480536
 H11       0.8137516468      1.3748090643      3.2295507584
 H12       0.3771305267     -0.2499480191      3.7614906919
 H13      -0.7663915561      1.0701501320      3.9568907157

 nuclear repulsion energy.......  1414.909215676 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  26   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.333E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom         H1     C1      C2      C3      C4      C5      C6
C7
  grid # 1        72     87      89      90      89      88      84
81
  grid # 2       116     97      96      98      97      97      94
90
  grid # 3       217    182     184     194     183     184     189
177
  grid # 4       216    326     328     338     328     328     323
314

  number of gridpoints:
     atom         H3     H4      H6     C16      C8      N2      C9
C10
  grid # 1        73     73      70      92      82      95      82
69
  grid # 2       118    118     112     100      90     105      92
78
  grid # 3       223    223     207     194     174     211     176
147
  grid # 4       224    223     207     342     311     387     293
275

  number of gridpoints:
     atom         O1    C23     C18     C19     C20     C21     C22
H2
  grid # 1       111     74      89      88      88      89      89
71
  grid # 2       123     80      97      95      96      97      96
112
  grid # 3       257    149     183     183     182     184     183
212
  grid # 4       450    287     327     326     327     327     327
211

  number of gridpoints:
     atom         H5     H7      H8      H9     H10     H19     H20
H21
  grid # 1        71     73      73      73      67      71      71
70
  grid # 2       111    118     118     118     106     108     110
108
  grid # 3       212    223     223     224     202     218     216
217
  grid # 4       207    223     224     224     197     213     216
215

  number of gridpoints:
     atom        H22    H11     H12     H13  total
```

```
  grid # 1       69     71     70     71   2865
  grid # 2      110    109    107    111   3728
  grid # 3      214    214    212    217   7190
  grid # 4      211    211    209    218   9913

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d    total energy      change  change    error

etot   1  N  N  1  U  -783.03319876939           2.3E-05  5.8E-04
etot   2  Y  Y  4  M  -783.03323974059  4.1E-05  7.3E-06  2.3E-04
etot   3  Y  Y  4  M  -783.03324620964  6.5E-06  2.3E-06  6.5E-05
etot   4  Y  N  4  M  -783.03324605340 -1.6E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.90921567646
   (E)  Total one-electron terms..... -3874.38940440734
   (I)  Total two-electron terms.....  1676.44694267749
   (L)  Electronic energy............. -2197.94246172986  (E+I)
   (N)  Total energy.................  -783.03324605340  (A+L)

 SCFE: SCF energy: HF    -783.03324605340 hartrees   iterations:
4


 HOMO energy:    -0.30202
 LUMO energy:     0.12924

  Orbital energies:
  -20.52693  -15.60025  -11.34604  -11.28583  -11.25654  -11.24990
  -11.24307  -11.24142  -11.24051  -11.23864  -11.23787  -11.23485
  -11.23145  -11.23061  -11.23009  -11.22979  -11.22866  -11.22763
  -11.20921   -1.39734   -1.26949   -1.16507   -1.14896   -1.10601
   -1.03003   -1.01864   -1.01787   -1.01268   -0.96258   -0.93267
   -0.85809   -0.83887   -0.83328   -0.82168   -0.79606   -0.74108
   -0.71098   -0.69499   -0.67285   -0.66427   -0.64456   -0.63761
   -0.62742   -0.61487   -0.61225   -0.60856   -0.59703   -0.58332
   -0.57631   -0.55333   -0.54869   -0.54062   -0.53102   -0.51896
   -0.51491   -0.50720   -0.50099   -0.49777   -0.48459   -0.46861
   -0.46288   -0.42152   -0.41152   -0.34259   -0.33293   -0.32291
   -0.30202    0.12924    0.13403    0.14449    0.15237    0.20394
```

0.22970 0.24103 0.24873 0.26129 0.28798

end of program scf

start of program der1a
end of program der1a

start of program rwr
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	-1.792178E-05	2.698075E-05	9.931760E-06
2	C1	-4.199006E-05	2.670115E-05	-6.619590E-05
3	C2	-8.823182E-05	1.499805E-04	5.690472E-05
4	C3	1.579278E-05	-6.367312E-05	-7.640469E-05
5	C4	-1.255170E-05	1.367502E-04	6.529504E-05
6	C5	-4.801133E-05	9.386148E-05	-6.154220E-05
7	C6	2.006852E-04	-1.277318E-04	7.927641E-05
8	C7	-1.934084E-04	4.005420E-05	-6.789881E-05
9	H3	-1.721716E-05	1.468154E-05	1.066046E-05
10	H4	-1.824596E-05	9.375496E-06	-1.374919E-05
11	H6	-4.016218E-05	5.683665E-05	-3.846933E-05
12	C16	-6.178309E-05	-1.417935E-04	-6.482654E-05
13	C8	1.979363E-04	7.852375E-05	4.670826E-05
14	N2	-2.080181E-04	-1.484989E-04	-8.149019E-04
15	C9	-1.070313E-04	1.479891E-04	4.834012E-04
16	C10	-1.226518E-05	-3.260580E-05	6.293867E-05
17	O1	4.586248E-05	2.250521E-04	-9.902369E-05
18	C23	9.323347E-05	-1.697030E-04	6.568540E-05
19	C18	-1.058083E-04	7.957653E-06	-6.525818E-05
20	C19	9.945809E-05	-7.383997E-06	-9.282804E-05
21	C20	1.053703E-04	-7.017946E-05	-9.893442E-05
22	C21	-5.107794E-05	7.666092E-05	-1.227864E-05
23	C22	-1.118093E-04	7.346956E-05	6.439589E-05
24	H2	6.428220E-05	5.038711E-05	6.818552E-05
25	H5	-3.915196E-05	1.808051E-04	1.147863E-04
26	H7	-3.490964E-05	3.468745E-05	-1.847892E-06
27	H8	-2.301831E-05	1.793970E-05	1.105163E-05
28	H9	-5.992197E-05	3.180286E-05	-2.453409E-06
29	H10	2.853175E-05	4.350199E-05	3.840084E-05
30	H19	-3.297343E-04	1.963730E-04	3.111567E-05
31	H20	-7.354949E-05	-2.253680E-05	3.250965E-05
32	H21	1.115962E-04	1.245728E-04	-2.175801E-04
33	H22	4.246882E-05	-3.002054E-05	-1.482063E-05

```
 34    H11    -1.123591E-04   8.593346E-05   6.140635E-05
 35    H12    -5.157430E-05  -7.412981E-05   6.178159E-05
 36    H13     1.116070E-04   1.554233E-05   1.800480E-04
-----------   -------------  -------------  -------------
   total      -7.429282E-04   1.058164E-03  -2.645302E-04

 end of program der1b


 start of program geopt  27

 geometry optimization step 27
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0102619
  Cos(theta):   0.6344988

  Final level shift:  -3.5962325E-02

 energy change:          -3.0792E-06 *  (  5.0000E-05 )
 gradient maximum:        8.2073E-04 .  (  4.5000E-04 )
 gradient rms:            1.5112E-04 *  (  3.0000E-04 )
 step size:   0.01026  trust radius:   0.01000
 displacement maximum:    4.2285E-03 .  (  1.8000E-03 )
 displacement rms:        9.2907E-04 *  (  1.2000E-03 )
 predicted energy change:    -7.3276E-06    geom step:   1.0262E-
02    full step:   1.0262E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:     1.0470E-03     y:     1.2433E-04     z:    -4.8036E-04

 new geometry:
                                 angstroms
 atom            x                  y                  z
 H1       -1.1794720243      1.8871569488     -2.2321788095
 C1       -1.0972890597      2.1201593223     -1.1841642894
 C2       -0.8821948365      2.6957221129      1.5033551746
 C3       -0.8785521726      1.0863737601     -0.2888271952
 C4       -1.2019040261      3.4348576098     -0.7607198357
 C5       -1.0947227599      3.7145428017      0.5891824574
 C6       -0.7670616047      1.3774891464      1.0728390581
 C7       -0.7870699621     -0.3532015709     -0.7559934079
 H3       -1.3672413785      4.2232026877     -1.4727419145
 H4       -1.1804041545      4.7270911767      0.9422470827
 H6       -0.8134670244      2.9346878000      2.5466863749
 C16       0.6125854325     -0.7649482464     -1.2108724078
```

```
  C8       -1.3968720220     -1.2508271909      0.3434884075
  N2       -0.5109487517      0.3379567172      1.9938959639
  C9       -0.7808597944     -0.9773199102      1.7055047391
  C10       0.0017912188      0.6548980036      3.3194622764
  O1       -0.5778772296     -1.8515145469      2.5000402312
  C23      -1.3867054964     -2.7425504517      0.0244735751
  C18       3.1400102171     -1.5826522821     -2.0962098764
  C19       0.7602748837     -1.4841259595     -2.3917962659
  C20       1.7590355243     -0.4513129558     -0.4850209520
  C21       3.0083076079     -0.8592562788     -0.9209425995
  C22       2.0099080046     -1.8915889012     -2.8329894489
  H2       -0.1102272433     -1.7310312277     -2.9751269232
  H5        1.6832891008      0.1213768310      0.4207957459
  H7        3.8801859460     -0.6079136199     -0.3425947003
  H8        2.0970003175     -2.4471452223     -3.7503190464
  H9        4.1119248414     -1.8965030187     -2.4341384458
  H10      -1.4338253536     -0.4542944809     -1.6210529454
  H19      -0.3772496834     -3.1282609528     -0.0248868416
  H20      -1.8702424424     -2.9212139352     -0.9313669075
  H21      -1.9168614624     -3.2944639093      0.7881952227
  H22      -2.4339244095     -0.9274179933      0.4420104673
  H11       0.8079845370      1.3736044673      3.2378540602
  H12       0.3703125208     -0.2536724748      3.7634617095
  H13      -0.7733320429      1.0652918938      3.9595084252

  nuclear repulsion energy.......  1414.896885768 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  27   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
```

```
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    325
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
80
  grid # 3      223    223    207    194    174    211    176
144
  grid # 4      224    223    207    342    311    387    293
272

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     81     97     95     96     97     96
112
  grid # 3      256    145    183    183    182    184    183
212
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2861
  grid # 2      110    109    107    111   3732
  grid # 3      214    214    213    217   7185
  grid # 4      211    211    209    218   9909

  end of program grid


  start of program rwr
```

```
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS     maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  1  U  -783.03318666421             2.5E-05  8.9E-04
etot  2  Y  Y  4  M  -783.03324219424  5.6E-05  8.7E-06  3.5E-04
etot  3  Y  Y  4  M  -783.03324698572  4.8E-06  2.7E-06  9.4E-05
etot  4  Y  N  4  M  -783.03324679073 -1.9E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89688576840
   (E)  Total one-electron terms..... -3874.35979172694
   (I)  Total two-electron terms.....  1676.42965916780
   (L)  Electronic energy............. -2197.93013255913  (E+I)
   (N)  Total energy.................  -783.03324679073  (A+L)

 SCFE: SCF energy: HF    -783.03324679073 hartrees   iterations:
4


 HOMO energy:    -0.30203
 LUMO energy:     0.12926

  Orbital energies:
  -20.52671  -15.60056  -11.34609  -11.28618  -11.25663  -11.25003
  -11.24304  -11.24166  -11.24054  -11.23856  -11.23793  -11.23495
  -11.23119  -11.23054  -11.22999  -11.22952  -11.22850  -11.22778
  -11.20895   -1.39751   -1.26973   -1.16513   -1.14898   -1.10606
   -1.03011   -1.01866   -1.01790   -1.01272   -0.96259   -0.93279
   -0.85825   -0.83905   -0.83332   -0.82169   -0.79612   -0.74122
   -0.71103   -0.69500   -0.67290   -0.66432   -0.64464   -0.63756
   -0.62744   -0.61489   -0.61226   -0.60857   -0.59695   -0.58334
   -0.57634   -0.55334   -0.54885   -0.54071   -0.53105   -0.51906
   -0.51486   -0.50724   -0.50107   -0.49777   -0.48458   -0.46870
   -0.46286   -0.42170   -0.41157   -0.34262   -0.33294   -0.32290
   -0.30203    0.12926    0.13404    0.14449    0.15229    0.20392
    0.22978    0.24103    0.24891    0.26127    0.28813

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.090848E-05	4.081619E-05	-4.434719E-05
2	C1	-8.989497E-06	4.357245E-05	5.401417E-05
3	C2	-5.143640E-05	-1.093332E-04	-6.448534E-05
4	C3	1.847298E-06	1.145373E-04	1.040952E-04
5	C4	-2.015133E-05	-8.740820E-05	-8.751947E-05
6	C5	9.266937E-06	-2.638054E-05	4.224999E-05
7	C6	-1.366397E-04	2.251690E-04	-2.121963E-04
8	C7	1.189142E-04	4.867431E-05	4.540536E-05
9	H3	-2.657231E-05	6.823764E-05	-4.882791E-05
10	H4	-2.296779E-05	6.895143E-05	-8.812317E-06
11	H6	-1.258229E-05	1.241295E-05	2.908081E-05
12	C16	-3.674520E-05	2.678891E-04	1.310726E-04
13	C8	-1.375373E-04	-3.900588E-05	-9.435071E-05
14	N2	9.403301E-05	1.452120E-04	8.008472E-04
15	C9	-3.450005E-05	-4.602372E-05	-4.751891E-04
16	C10	1.649608E-05	-8.706207E-05	3.087787E-05
17	O1	-8.637606E-05	-5.641202E-05	1.305854E-04
18	C23	-1.445009E-04	2.742175E-04	-1.233591E-04
19	C18	1.590060E-04	4.030787E-05	3.857896E-05
20	C19	-1.360583E-04	2.680931E-05	7.445288E-06
21	C20	-1.194817E-04	1.964006E-04	1.927457E-04
22	C21	3.052576E-05	4.049398E-05	9.407518E-05
23	C22	2.349070E-06	-3.341260E-05	-1.113862E-04
24	H2	-1.580351E-04	-8.381589E-06	-1.438517E-04
25	H5	5.462735E-06	-1.678341E-04	-1.434524E-04
26	H7	3.340883E-06	1.092779E-05	5.767035E-06
27	H8	-1.946931E-05	-5.369301E-06	-1.201840E-04
28	H9	2.354580E-05	1.237455E-05	-2.718097E-05
29	H10	-8.440204E-05	5.228979E-06	-6.750030E-05
30	H19	3.304385E-04	-1.669095E-04	-2.966068E-05
31	H20	1.328988E-05	8.538985E-05	-7.738057E-05
32	H21	-1.835455E-04	-1.009555E-04	2.293352E-04
33	H22	-1.291988E-04	7.378964E-05	9.136342E-06
34	H11	-1.821911E-05	2.933369E-05	-6.064266E-05
35	H12	5.778679E-05	1.833578E-04	-7.720539E-05
36	H13	-3.584516E-05	-1.437868E-05	-2.293819E-04
total		-7.578594E-04	1.065237E-03	-3.016019E-04

```
 end of program der1b
```

```
 start of program geopt  28

 geometry optimization step 28
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0101973
  Cos(theta):   0.7537542

  Final level shift:  -6.9111039E-02

 energy change:          -7.3734E-07 #  (  5.0000E-05 )
 gradient maximum:        5.2607E-04 .  (  4.5000E-04 )
 gradient rms:            1.5503E-04 *  (  3.0000E-04 )
 step size:   0.01020  trust radius:   0.01000
 displacement maximum:    4.1528E-03 .  (  1.8000E-03 )
 displacement rms:        9.2322E-04 *  (  1.2000E-03 )
 predicted energy change:    -1.0174E-05    geom step:   1.0197E-
02    full step:   1.0197E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -9.6132E-04     y:     7.3494E-05     z:     4.2561E-04

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1803715093     1.8862877194    -2.2324771278
 C1       -1.0985303416     2.1196351010    -1.1844611373
 C2       -0.8838817211     2.6957482142     1.5028513354
 C3       -0.8794531353     1.0863604536    -0.2886923671
 C4       -1.2037681891     3.4342116441    -0.7615119703
 C5       -1.0967006381     3.7142365264     0.5884150832
 C6       -0.7683622701     1.3776901146     1.0727258012
 C7       -0.7870035225    -0.3530466722    -0.7559180889
 H3       -1.3693523761     4.2223805246    -1.4737992268
 H4       -1.1827758026     4.7269341414     0.9411067211
 H6       -0.8150175337     2.9346929253     2.5462543717
 C16       0.6127588524    -0.7640467225    -1.2106833025
 C8       -1.3972405500    -1.2509129913     0.3431601902
 N2       -0.5106132583     0.3384239096     1.9944478262
 C9       -0.7809295348    -0.9770557626     1.7051378013
 C10       0.0071783429     0.6572169777     3.3167850463
 O1       -0.5786036552    -1.8510309033     2.5001725757
 C23      -1.3852046176    -2.7427410246     0.0247723685
 C18       3.1404609695    -1.5837747157    -2.0948055187
 C19       0.7609331817    -1.4789741050    -2.3945435036
 C20       1.7585428783    -0.4566955416    -0.4809682830
```

```
  C21       3.0079416483     -0.8655994230     -0.9162914807
  C22       2.0108545244     -1.8870764343     -2.8352920419
  H2       -0.1092190569     -1.7221972031     -2.9807795296
  H5        1.6823121655      0.1097058269      0.4281009265
  H7        3.8792010646     -0.6190909500     -0.3349808891
  H8        2.0984099613     -2.4387891203     -3.7551383275
  H9        4.1123811988     -1.8982677948     -2.4323259928
  H10      -1.4337590168     -0.4544798159     -1.6211872382
  H19      -0.3749109308     -3.1292634445     -0.0201343286
  H20      -1.8638739371     -2.9210371349     -0.9336206240
  H21      -1.9192549809     -3.2946083017      0.7867341161
  H22      -2.4346069675     -0.9278921550      0.4413733792
  H11       0.8120954398      1.3769625698      3.2302258113
  H12       0.3798025486     -0.2495079542      3.7603695116
  H13      -0.7668205736      1.0673975340      3.9579282214

  nuclear repulsion energy.......  1414.900958421 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  28   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.333E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
```

```
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
147
  grid # 4      224    223    207    342    311    387    293
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2865
  grid # 2      110    109    107    111   3728
  grid # 3      214    214    212    217   7190
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
```

```
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -783.03319039242           2.0E-05  9.4E-04
etot   2  Y  Y  4  M  -783.03325183750  6.1E-05  9.0E-06  3.7E-04
etot   3  Y  Y  4  M  -783.03326266595  1.1E-05  2.9E-06  9.8E-05
etot   4  Y  N  4  M  -783.03326209570 -5.7E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.90095842069
   (E)  Total one-electron terms..... -3874.37436872279
   (I)  Total two-electron terms.....  1676.44014820640
   (L)  Electronic energy............. -2197.93422051639  (E+I)
   (N)  Total energy.................  -783.03326209570  (A+L)

 SCFE: SCF energy: HF    -783.03326209570 hartrees   iterations:
4


 HOMO energy:    -0.30201
 LUMO energy:     0.12926

  Orbital energies:
  -20.52693  -15.60020  -11.34596  -11.28579  -11.25655  -11.24984
  -11.24303  -11.24137  -11.24049  -11.23866  -11.23787  -11.23487
  -11.23146  -11.23060  -11.23011  -11.22980  -11.22867  -11.22760
  -11.20922   -1.39740   -1.26947   -1.16503   -1.14894   -1.10599
   -1.03002   -1.01863   -1.01783   -1.01268   -0.96257   -0.93266
   -0.85809   -0.83888   -0.83326   -0.82166   -0.79605   -0.74108
   -0.71097   -0.69498   -0.67284   -0.66427   -0.64456   -0.63757
   -0.62742   -0.61486   -0.61225   -0.60853   -0.59700   -0.58332
   -0.57628   -0.55333   -0.54870   -0.54064   -0.53102   -0.51898
   -0.51490   -0.50719   -0.50097   -0.49775   -0.48458   -0.46861
   -0.46286   -0.42152   -0.41152   -0.34256   -0.33293   -0.32287
   -0.30201    0.12926    0.13403    0.14450    0.15238    0.20393
    0.22970    0.24104    0.24874    0.26135    0.28818

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.555058E-05	2.235707E-05	2.128014E-05
2	C1	-3.883467E-05	5.426406E-05	-7.943889E-05
3	C2	-8.008048E-05	1.607169E-04	4.014778E-05
4	C3	4.816982E-07	-4.391354E-05	-1.421456E-04
5	C4	-1.725269E-05	1.229808E-04	5.752323E-05
6	C5	-3.922899E-05	8.383047E-05	-4.310034E-05
7	C6	1.624181E-04	-7.797360E-05	1.143179E-04
8	C7	-1.561167E-04	2.660171E-06	-8.892253E-05
9	H3	-7.793564E-06	-8.158132E-06	3.157353E-05
10	H4	-1.154392E-05	-1.359147E-05	-1.254950E-05
11	H6	-3.474480E-05	4.945667E-05	-4.642687E-05
12	C16	-6.624352E-05	-1.887955E-04	-7.234874E-05
13	C8	2.028370E-04	6.663933E-05	5.167696E-05
14	N2	-1.674183E-04	7.750970E-05	-6.419616E-04
15	C9	-1.084077E-04	1.281298E-04	3.696466E-04
16	C10	6.555533E-06	4.686658E-05	6.690168E-06
17	O1	3.102297E-05	2.302475E-05	-1.190399E-05
18	C23	5.140563E-05	-7.752578E-05	3.013557E-05
19	C18	-1.272726E-04	2.587652E-05	-6.504276E-05
20	C19	2.695637E-05	3.247964E-05	-4.844918E-05
21	C20	2.368255E-05	-1.534732E-04	-2.145792E-04
22	C21	-7.976129E-05	2.631499E-05	-1.101896E-04
23	C22	-4.969126E-05	5.482464E-05	6.399814E-05
24	H2	1.155120E-04	8.271584E-05	1.210675E-04
25	H5	-3.352982E-05	2.408379E-04	1.489408E-04
26	H7	7.638167E-06	5.572164E-05	6.592154E-06
27	H8	-1.973847E-05	4.631456E-05	8.901697E-05
28	H9	-4.629427E-05	4.658814E-05	6.399982E-06
29	H10	3.653094E-05	5.443721E-05	3.054239E-05
30	H19	-2.151140E-04	1.525051E-04	1.978718E-05
31	H20	-6.676981E-05	-5.047967E-06	1.707747E-05
32	H21	7.557822E-05	8.945987E-05	-1.679852E-04
33	H22	1.265353E-06	6.778123E-06	-7.898931E-06
34	H11	-1.377163E-04	3.926101E-05	3.184657E-05
35	H12	-3.607236E-05	-1.112579E-04	6.496164E-05
36	H13	8.648322E-05	6.846773E-06	1.326019E-04
total		-7.268083E-04	1.119661E-03	-2.971185E-04

```
 end of program der1b


 start of program geopt  29

 geometry optimization step 29
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
```

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0106921
   Cos(theta):   0.6480668

   Final level shift:  -4.3295903E-02

  energy change:          -1.5305E-05 *  (  5.0000E-05 )
  gradient maximum:        7.5522E-04 .  (  4.5000E-04 )
  gradient rms:            1.4572E-04 *  (  3.0000E-04 )
  step size:   0.01069  trust radius:   0.01000
  displacement maximum:    5.8680E-03 .  (  1.8000E-03 )
  displacement rms:        9.6802E-04 *  (  1.2000E-03 )
  predicted energy change:    -8.0511E-06    geom step:   1.0692E-
02    full step:   1.0692E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     6.2837E-04     y:    -1.0934E-04     z:    -2.7042E-04

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1788733885     1.8878718807    -2.2321586842
  C1       -1.0969269115     2.1206372364    -1.1840824746
  C2       -0.8825613167     2.6955463734     1.5037118382
  C3       -0.8783831535     1.0866648763    -0.2889295994
  C4       -1.2016150744     3.4351888220    -0.7602818654
  C5       -1.0948420529     3.7145587110     0.5897355743
  C6       -0.7671428566     1.3775024297     1.0728528398
  C7       -0.7869120089    -0.3528705335    -0.7562639684
  H3       -1.3667034600     4.2237130208    -1.4721255323
  H4       -1.1806502159     4.7270038069     0.9430156885
  H6       -0.8141699837     2.9341484341     2.5471452723
  C16       0.6127246537    -0.7649451979    -1.2107379449
  C8       -1.3972490390    -1.2504998139     0.3429472432
  N2       -0.5108322576     0.3378002355     1.9937562274
  C9       -0.7816101143    -0.9774533446     1.7052295352
  C10       0.0032617333     0.6542556842     3.3187332041
  O1       -0.5797565326    -1.8519107826     2.4999079573
  C23      -1.3870637865    -2.7421323603     0.0235852330
  C18       3.1403833217    -1.5828599247    -2.0956337379
  C19       0.7604488217    -1.4857920762    -2.3905652742
  C20       1.7592324781    -0.4497017897    -0.4858780360
  C21       3.0086124301    -0.8576395062    -0.9216005653
  C22       2.0101670655    -1.8935379538    -2.8314359855
  H2       -0.1100614100    -1.7338114890    -2.9732231543
  H5        1.6835999496     0.1246347759     0.4190201094
  H7        3.8806210858    -0.6047262352    -0.3440256644
  H8        2.0972348631    -2.4505899926    -3.7477444871
  H9        4.1123991701    -1.8966879647    -2.4333251864
  H10      -1.4334139749    -0.4537104506    -1.6215544736
```

```
  H19      -0.3774696748     -3.1281547414     -0.0251899498
  H20      -1.8698920370     -2.9203376809     -0.9327199536
  H21      -1.9179220104     -3.2942602638      0.7868296311
  H22      -2.4343657864     -0.9269015691      0.4412054956
  H11       0.8079407585      1.3743923393      3.2364059946
  H12       0.3742016284     -0.2540835313      3.7613795805
  H13      -0.7717628830      1.0625676536      3.9601168675

  nuclear repulsion energy.......  1414.898785614 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  29   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    325
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
80
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    207    342    311    387    293
272
```

```
  number of gridpoints:
     atom         O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1       111     73     89     88     88     89     89
71
  grid # 2       123     80     97     95     96     97     96
112
  grid # 3       256    147    183    183    182    184    183
212
  grid # 4       450    285    327    326    327    327    327
211

  number of gridpoints:
     atom         H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1        71     73     73     73     66     71     71
70
  grid # 2       111    118    118    118    106    108    110
108
  grid # 3       212    223    223    224    203    218    217
217
  grid # 4       207    223    224    224    196    212    216
215

  number of gridpoints:
     atom        H22    H11    H12    H13  total
  grid # 1        69     71     70     71   2862
  grid # 2       110    109    107    111   3731
  grid # 3       214    214    213    217   7186
  grid # 4       211    211    209    218   9908

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy       change  change    error

etot   1  N  N  1  U  -783.03315216126                2.3E-05  1.2E-03
etot   2  Y  Y  4  M  -783.03324048549  8.8E-05  1.1E-05  4.9E-04
etot   3  Y  Y  4  M  -783.03325036853  9.9E-06  3.4E-06  1.2E-04
etot   4  Y  N  4  M  -783.03325250590  2.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
```

```
   (A)  Nuclear repulsion.....  1414.89878561400
   (E)  Total one-electron terms..... -3874.36244561246
   (I)  Total two-electron terms.....  1676.43040749256
   (L)  Electronic energy..... -2197.93203811990  (E+I)
   (N)  Total energy.............  -783.03325250590  (A+L)

 SCFE: SCF energy: HF    -783.03325250590 hartrees   iterations:
4


 HOMO energy:    -0.30206
 LUMO energy:     0.12927

  Orbital energies:
 -20.52667  -15.60060  -11.34615  -11.28622  -11.25662  -11.25007
 -11.24309  -11.24172  -11.24054  -11.23854  -11.23793  -11.23494
 -11.23116  -11.23053  -11.22998  -11.22950  -11.22848  -11.22781
 -11.20900   -1.39743   -1.26973   -1.16516   -1.14900   -1.10608
  -1.03013   -1.01868   -1.01793   -1.01271   -0.96259   -0.93280
  -0.85825   -0.83904   -0.83335   -0.82171   -0.79613   -0.74122
  -0.71103   -0.69501   -0.67290   -0.66434   -0.64465   -0.63757
  -0.62744   -0.61490   -0.61226   -0.60860   -0.59696   -0.58332
  -0.57637   -0.55339   -0.54884   -0.54071   -0.53103   -0.51906
  -0.51484   -0.50724   -0.50109   -0.49778   -0.48458   -0.46870
  -0.46288   -0.42169   -0.41157   -0.34264   -0.33293   -0.32294
  -0.30206    0.12927    0.13405    0.14446    0.15226    0.20389
   0.22976    0.24100    0.24891    0.26128    0.28813

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x             y             z
 ----  -----   -------------  -------------  -------------
   1    H1     -2.291875E-05   4.619516E-05  -5.526117E-05
   2    C1     -6.479568E-06   6.184105E-06   7.165012E-05
   3    C2     -4.165763E-05  -1.158589E-04  -5.670997E-05
   4    C3      1.783000E-05   9.688100E-05   1.558037E-04
   5    C4     -2.068571E-05  -6.135089E-05  -7.741331E-05
   6    C5      1.916573E-06  -1.235763E-05   2.501196E-05
   7    C6     -1.036172E-04   1.575757E-04  -2.246117E-04
```

```
 8    C7      8.084306E-05   7.878387E-05   6.507889E-05
 9    H3     -3.608134E-05   8.944618E-05  -6.485638E-05
10    H4     -2.957888E-05   8.858321E-05  -7.074376E-06
11    H6     -1.648444E-05   2.255296E-05   4.057173E-05
12    C16    -2.331645E-05   3.153548E-04   1.221708E-04
13    C8     -1.561792E-04  -1.890658E-05  -7.369775E-05
14    N2      4.857373E-05  -9.977499E-05   5.748698E-04
15    C9     -2.490452E-05  -7.974711E-06  -3.380531E-04
16    C10    -1.102960E-05  -1.691847E-04   7.056659E-05
17    O1     -6.380146E-05   1.387361E-04   2.029738E-05
18    C23    -9.872603E-05   1.616321E-04  -8.066078E-05
19    C18     1.735218E-04   2.690809E-05   3.523366E-05
20    C19    -4.715140E-05  -2.108353E-05  -2.587199E-05
21    C20    -3.829152E-05   2.837459E-04   3.182249E-04
22    C21     6.012526E-05   9.623631E-05   1.959838E-04
23    C22    -7.883133E-05  -2.672005E-06  -9.565389E-05
24    H2     -2.094142E-04  -3.414577E-05  -2.029990E-04
25    H5      5.249878E-06  -2.252649E-04  -1.966494E-04
26    H7     -3.735866E-05  -8.355032E-06   8.551318E-07
27    H8     -2.544330E-05  -3.346991E-05  -1.985792E-04
28    H9      1.322562E-05   2.225875E-06  -3.526835E-05
29    H10    -8.571758E-05  -1.738086E-06  -6.171350E-05
30    H19     1.923556E-04  -1.050529E-04  -2.424592E-05
31    H20     7.966574E-06   6.361570E-05  -5.888849E-05
32    H21    -1.399424E-04  -6.214505E-05   1.656624E-04
33    H22    -6.928268E-05   3.972374E-05  -1.163258E-06
34    H11     3.711121E-05   8.676907E-05  -3.379518E-05
35    H12     2.414597E-05   2.112359E-04  -8.316705E-05
36    H13    -3.403679E-05   1.505834E-05  -1.490863E-04
-----------   -------------  -------------  -------------
   total      -7.580653E-04   1.048109E-03  -2.834393E-04

 end of program der1b


 start of program geopt  30

 geometry optimization step 30
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0102779
  Cos(theta):   0.7505295

  Final level shift:  -7.0341646E-02

 energy change:           9.5898E-06 *  (  5.0000E-05 )
 gradient maximum:        6.9613E-04 .  (  4.5000E-04 )
```

```
  gradient rms:            1.5767E-04 *  (  3.0000E-04 )
  step size:   0.01028  trust radius:   0.01000
  displacement maximum:    5.2263E-03 .  (  1.8000E-03 )
  displacement rms:        9.3052E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0432E-05    geom step:   1.0278E-
02    full step:   1.0278E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -5.7134E-04     y:     2.5290E-04     z:     2.3719E-04

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1805123374     1.8867936054    -2.2324492312
  C1       -1.0987022558     2.1199966291    -1.1843885336
  C2       -0.8843825584     2.6957770680     1.5030058967
  C3       -0.8792396632     1.0866573611    -0.2887712064
  C4       -1.2044006184     3.4345052928    -0.7612731570
  C5       -1.0975679291     3.7143600833     0.5887152380
  C6       -0.7681579294     1.3778353300     1.0726376556
  C7       -0.7867729005    -0.3526760767    -0.7561339119
  H3       -1.3702777808     4.2227221699    -1.4734774897
  H4       -1.1841535528     4.7269811065     0.9415477882
  H6       -0.8158280791     2.9345404458     2.5464881850
  C16       0.6129672682    -0.7638347851    -1.2107899090
  C8       -1.3970719193    -1.2506771706     0.3428740029
  N2       -0.5101316193     0.3384333396     1.9940885887
  C9       -0.7808855476    -0.9768080678     1.7049086498
  C10       0.0076980643     0.6568999616     3.3166329033
  O1       -0.5787381399    -1.8505929524     2.5000946720
  C23      -1.3851990770    -2.7424650809     0.0243381872
  C18       3.1404059156    -1.5847881970    -2.0943049621
  C19       0.7609888794    -1.4793841273    -2.3943718788
  C20       1.7587886750    -0.4564976935    -0.4810318407
  C21       3.0080832709    -0.8660365856    -0.9160622612
  C22       2.0107577591    -1.8880458188    -2.8348320802
  H2       -0.1092374759    -1.7227952576    -2.9805504868
  H5        1.6825896955     0.1100065804     0.4278922490
  H7        3.8793407938    -0.6196926036    -0.3347464705
  H8        2.0981974813    -2.4402295888    -3.7544900465
  H9        4.1122043722    -1.8998594056    -2.4316268240
  H10      -1.4335227037    -0.4540695253    -1.6214064104
  H19      -0.3749732186    -3.1288677070    -0.0210363964
  H20      -1.8643494741    -2.9207585335    -0.9338201340
  H21      -1.9188234392    -3.2944596906     0.7864235050
  H22      -2.4344262036    -0.9277216856     0.4410460566
  H11       0.8111674768     1.3783551672     3.2304635014
  H12       0.3822797976    -0.2495114785     3.7591361978
  H13      -0.7665827175     1.0649690285     3.9588532714

  nuclear repulsion energy.......  1414.900937188 hartrees
```

```
  ------------------------------------------------
 /  end of geometry optimization iteration  30   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.333E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
147
  grid # 4      224    223    207    342    311    387    293
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
```

```
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2865
  grid # 2      110    109    107    111   3728
  grid # 3      214    214    212    217   7190
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                              energy  density   DIIS
       e  d  i  u  i                              change  change    error
       r  t  s  t  d     total energy

etot   1  N  N  1  U  -783.03316267992                    2.3E-05  1.2E-03
etot   2  Y  Y  4  M  -783.03324716945  8.4E-05  1.1E-05  4.7E-04
etot   3  Y  Y  4  M  -783.03326193495  1.5E-05  3.4E-06  1.2E-04
etot   4  Y  N  4  M  -783.03326085436 -1.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.90093718834
   (E)  Total one-electron terms..... -3874.37502559364
   (I)  Total two-electron terms.....  1676.44082755094
   (L)  Electronic energy............. -2197.93419804270  (E+I)
   (N)  Total energy.................  -783.03326085436  (A+L)

 SCFE: SCF energy: HF    -783.03326085436 hartrees   iterations:
4
```

```
HOMO energy:    -0.30202
LUMO energy:     0.12927

 Orbital energies:
 -20.52693  -15.60015  -11.34589  -11.28577  -11.25657  -11.24982
 -11.24300  -11.24134  -11.24049  -11.23869  -11.23788  -11.23489
 -11.23147  -11.23060  -11.23013  -11.22981  -11.22868  -11.22759
 -11.20920   -1.39744   -1.26945   -1.16501   -1.14893   -1.10597
  -1.03001   -1.01862   -1.01781   -1.01269   -0.96256   -0.93266
  -0.85808   -0.83889   -0.83326   -0.82165   -0.79604   -0.74108
  -0.71095   -0.69497   -0.67283   -0.66426   -0.64456   -0.63755
  -0.62742   -0.61486   -0.61225   -0.60851   -0.59697   -0.58334
  -0.57626   -0.55334   -0.54870   -0.54064   -0.53101   -0.51901
  -0.51489   -0.50718   -0.50097   -0.49775   -0.48457   -0.46861
  -0.46285   -0.42151   -0.41151   -0.34255   -0.33293   -0.32285
  -0.30202    0.12927    0.13403    0.14450    0.15237    0.20396
   0.22970    0.24104    0.24878    0.26135    0.28821

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H1     -1.426589E-05   1.851512E-05   3.087180E-05
  2    C1     -3.684092E-05   8.102257E-05  -9.089714E-05
  3    C2     -8.044580E-05   1.582930E-04   4.084435E-05
  4    C3     -1.664687E-05  -2.696388E-05  -1.842010E-04
  5    C4     -1.838719E-05   1.079364E-04   5.562918E-05
  6    C5     -3.254149E-05   6.980998E-05  -3.444434E-05
  7    C6      1.237987E-04  -3.684853E-05   1.446596E-04
  8    C7     -1.452748E-04  -3.450633E-05  -7.213955E-05
  9    H3     -7.641201E-07  -2.547748E-05   4.682395E-05
 10    H4     -7.293925E-06  -3.079856E-05  -1.251058E-05
 11    H6     -3.496943E-05   4.155554E-05  -5.383499E-05
 12    C16    -5.004429E-05  -2.187798E-04  -8.074203E-05
 13    C8      1.725416E-04   8.367618E-05   3.420425E-05
 14    N2     -1.302220E-04   2.592129E-04  -5.062677E-04
 15    C9     -9.589599E-05   9.124701E-05   2.739530E-04
 16    C10     1.282326E-05   1.094053E-04  -1.801434E-05
```

```
 17    O1      1.872458E-05  -1.381686E-04   6.135473E-05
 18    C23     4.559994E-05  -5.292458E-05   1.914318E-05
 19    C18    -1.373014E-04   3.592146E-05  -5.941809E-05
 20    C19    -4.120612E-05   5.938575E-05  -1.533590E-05
 21    C20    -2.492204E-05  -2.159300E-04  -2.948217E-04
 22    C21    -1.035986E-04  -1.029270E-05  -1.834305E-04
 23    C22     1.698841E-05   3.331820E-05   4.922204E-05
 24    H2      1.502027E-04   1.049101E-04   1.597948E-04
 25    H5     -3.682739E-05   2.895247E-04   1.828157E-04
 26    H7      3.172094E-05   6.790982E-05   1.109181E-05
 27    H8     -1.532688E-05   6.759531E-05   1.418245E-04
 28    H9     -4.032796E-05   5.556332E-05   1.230163E-05
 29    H10     4.007010E-05   6.090349E-05   2.669803E-05
 30    H19    -1.590801E-04   1.191706E-04   1.113621E-05
 31    H20    -5.356989E-05   9.065189E-06   1.585560E-05
 32    H21     5.125398E-05   8.272473E-05  -1.302354E-04
 33    H22    -2.098380E-05   3.016177E-05  -5.339662E-06
 34    H11    -1.555313E-04  -1.591497E-06   4.876376E-06
 35    H12    -2.306733E-05  -1.300998E-04   6.292347E-05
 36    H13     7.240151E-05  -6.950884E-06   6.617608E-05
-----------   -------------  -------------  -------------
   total      -7.392099E-04   1.107496E-03  -2.894327E-04

 end of program der1b


 start of program geopt  31

 geometry optimization step 31
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0101118
  Cos(theta):   0.6906135

  Final level shift:  -5.5148463E-02

 energy change:          -8.3485E-06 *  (  5.0000E-05 )
 gradient maximum:        7.1732E-04 .  (  4.5000E-04 )
 gradient rms:            1.5254E-04 *  (  3.0000E-04 )
 step size:   0.01011  trust radius:   0.01000
 displacement maximum:    5.8173E-03 .  (  1.8000E-03 )
 displacement rms:        9.1548E-04 *  (  1.2000E-03 )
 predicted energy change:    -8.7025E-06    geom step:   1.0112E-
02    full step:   1.0112E-02
 molecular structure not yet converged...

 center of mass moved by:
```

x: 2.9380E-04 y: -2.7459E-04 z: -1.1282E-04

new geometry:

atom	x	y	z
		angstroms	
H1	-1.1784744123	1.8882686829	-2.2322594255
C1	-1.0967446034	2.1208831420	-1.1841335713
C2	-0.8830373084	2.6953892194	1.5038482133
C3	-0.8783475037	1.0868126030	-0.2890727080
C4	-1.2015304023	3.4353320382	-0.7601208114
C5	-1.0951307495	3.7145049023	0.5899771324
C6	-0.7673169578	1.3774970381	1.0727614418
C7	-0.7868439381	-0.3527298733	-0.7564234333
H3	-1.3664262171	4.2239737886	-1.4718630474
H4	-1.1810954908	4.7268859831	0.9433773969
H6	-0.8149588001	2.9337410893	2.5473698676
C16	0.6128511509	-0.7649325879	-1.2105679736
C8	-1.3976156064	-1.2503023581	0.3426200054
N2	-0.5106931159	0.3377130855	1.9935686305
C9	-0.7821390684	-0.9775165660	1.7050335478
C10	0.0048942744	0.6539187767	3.3178642090
O1	-0.5809843376	-1.8520860195	2.4998650317
C23	-1.3875177400	-2.7419672636	0.0232398106
C18	3.1407294868	-1.5828826129	-2.0950773323
C19	0.7606971708	-1.4863862054	-2.3900044755
C20	1.7592997626	-0.4491332063	-0.4859378804
C21	3.0087791720	-0.8570290192	-0.9214878133
C22	2.0105218153	-1.8942323263	-2.8306348223
H2	-0.1097528079	-1.7347063758	-2.9725726183
H5	1.6836488840	0.1258064947	0.4186229251
H7	3.8807931579	-0.6035270362	-0.3441030183
H8	2.0976672541	-2.4518383725	-3.7465653319
H9	4.1128405038	-1.8966485085	-2.4325954368
H10	-1.4331399944	-0.4534524564	-1.6219120036
H19	-0.3778783778	-3.1284374996	-0.0247114455
H20	-1.8695078423	-2.9198717239	-0.9335613779
H21	-1.9193041409	-3.2939911842	0.7860854492
H22	-2.4347534552	-0.9265059201	0.4406753525
H11	0.8083771744	1.3751915459	3.2345944718
H12	0.3778997877	-0.2541376147	3.7594204689
H13	-0.7698714217	1.0606886361	3.9604132089

nuclear repulsion energy..... 1414.901924449 hartrees

/ end of geometry optimization iteration 31 /

---

end of program geopt

start of program onee

smallest eigenvalue of S: 3.335E-04

```
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    325
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
80
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    207    342    311    387    293
272

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     73     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      256    148    183    183    182    184    183
212
  grid # 4      450    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
```

```
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2862
  grid # 2      110    109    107    111   3730
  grid # 3      214    214    213    217   7187
  grid # 4      211    211    209    218   9910

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03314183079           2.3E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03323427007  9.2E-05  1.1E-05  5.1E-04
etot   3  Y  Y  4  M  -783.03324530875  1.1E-05  3.5E-06  1.3E-04
etot   4  Y  N  4  M  -783.03324859431  3.3E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.90192444893
   (E)  Total one-electron terms..... -3874.36872250592
   (I)  Total two-electron terms.....  1676.43354946267
   (L)  Electronic energy............. -2197.93517304324  (E+I)
   (N)  Total energy.................  -783.03324859431  (A+L)

 SCFE: SCF energy: HF    -783.03324859431 hartrees   iterations:
4


 HOMO energy:    -0.30208
 LUMO energy:     0.12928

  Orbital energies:
  -20.52666  -15.60059  -11.34617  -11.28621  -11.25660  -11.25008
  -11.24312  -11.24173  -11.24054  -11.23854  -11.23794  -11.23494
  -11.23118  -11.23054  -11.22998  -11.22951  -11.22849  -11.22780
```

```
-11.20904   -1.39737   -1.26972   -1.16517   -1.14901   -1.10608
 -1.03013   -1.01869   -1.01794   -1.01270   -0.96259   -0.93279
 -0.85824   -0.83902   -0.83336   -0.82171   -0.79613   -0.74122
 -0.71102   -0.69502   -0.67288   -0.66434   -0.64466   -0.63757
 -0.62743   -0.61491   -0.61226   -0.60861   -0.59695   -0.58331
 -0.57638   -0.55341   -0.54884   -0.54070   -0.53100   -0.51904
 -0.51484   -0.50724   -0.50110   -0.49778   -0.48458   -0.46869
 -0.46289   -0.42166   -0.41156   -0.34265   -0.33293   -0.32295
 -0.30208    0.12928    0.13405    0.14444    0.15225    0.20386
  0.22975    0.24098    0.24890    0.26128    0.28808

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.404742E-05	4.754667E-05	-5.579707E-05
2	C1	-9.904101E-06	-1.436199E-05	6.727049E-05
3	C2	-3.461521E-05	-1.041731E-04	-4.711985E-05
4	C3	2.227234E-05	7.161678E-05	1.778311E-04
5	C4	-2.171104E-05	-3.543799E-05	-6.650890E-05
6	C5	-8.482687E-06	4.211565E-06	9.650904E-06
7	C6	-6.561724E-05	1.017547E-04	-2.094072E-04
8	C7	5.568391E-05	9.659257E-05	5.633930E-05
9	H3	-4.124406E-05	9.581958E-05	-6.999536E-05
10	H4	-3.323500E-05	9.574344E-05	-6.826367E-06
11	H6	-1.672949E-05	2.761841E-05	4.072736E-05
12	C16	-3.276049E-05	3.124763E-04	1.021785E-04
13	C8	-1.500623E-04	-3.081351E-05	-5.916262E-05
14	N2	8.524857E-06	-2.576460E-04	3.772233E-04
15	C9	-1.787851E-05	2.106387E-05	-2.125153E-04
16	C10	-1.850964E-05	-1.984251E-04	8.167635E-05
17	O1	-4.860174E-05	2.642578E-04	-6.242037E-05
18	C23	-6.418195E-05	9.729238E-05	-4.928060E-05
19	C18	1.517736E-04	1.543276E-05	2.632914E-05
20	C19	1.828600E-05	-3.257051E-05	-4.238181E-05
21	C20	3.879775E-06	3.184401E-04	3.605515E-04
22	C21	8.513977E-05	1.128959E-04	2.290449E-04
23	C22	-1.162292E-04	2.048146E-05	-7.562564E-05
24	H2	-2.195842E-04	-4.722278E-05	-2.136909E-04

```
 25    H5      1.202067E-06  -2.483266E-04  -2.179985E-04
 26    H7     -6.505745E-05  -1.791902E-05  -6.458551E-06
 27    H8     -2.704162E-05  -3.839012E-05  -2.191198E-04
 28    H9      9.522707E-08  -1.786897E-06  -3.456762E-05
 29    H10    -7.719892E-05  -4.181916E-06  -4.876142E-05
 30    H19     7.990887E-05  -4.540067E-05  -1.182281E-05
 31    H20     6.020711E-07   4.309701E-05  -3.990120E-05
 32    H21    -9.219832E-05  -2.416461E-05   9.527453E-05
 33    H22    -2.795877E-05   1.804357E-05  -8.307698E-06
 34    H11     6.067803E-05   1.184266E-04  -8.954794E-06
 35    H12    -1.145550E-06   2.112025E-04  -7.644332E-05
 36    H13    -3.296717E-05   4.069534E-05  -6.754898E-05
-----------   -------------  -------------  -------------
   total      -7.589155E-04   1.033889E-03  -2.865194E-04

 end of program der1b


 start of program geopt  32

 geometry optimization step 32
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0102773
  Cos(theta):   0.7376274

  Final level shift:  -6.8396735E-02

 energy change:           1.2260E-05 *  (  5.0000E-05 )
 gradient maximum:        7.8834E-04 .  (  4.5000E-04 )
 gradient rms:            1.5954E-04 *  (  3.0000E-04 )
 step size:   0.01028  trust radius:   0.01000
 displacement maximum:    5.7136E-03 .  (  1.8000E-03 )
 displacement rms:        9.3046E-04 *  (  1.2000E-03 )
 predicted energy change:    -1.0292E-05    geom step:   1.0277E-
02    full step:   1.0277E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -2.9503E-04     y:     3.6280E-04     z:     9.8901E-05

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1805469221     1.8871065150    -2.2325080955
 C1       -1.0988018271     2.1202148201    -1.1844178494
 C2       -0.8848399873     2.6957931242     1.5030543100
```

```
 C3       -0.8790852409      1.0868307254     -0.2888915767
 C4       -1.2048523630      3.4346778980     -0.7611763057
 C5       -1.0982645768      3.7144259083      0.5888494252
 C6       -0.7680390380      1.3779370274      1.0725165604
 C7       -0.7866142635     -0.3524915012     -0.7562610005
 H3       -1.3709022057      4.2229251928     -1.4733231220
 H4       -1.1852497070      4.7269863058      0.9417739198
 H6       -0.8165507445      2.9344238949      2.5465994659
 C16       0.6131272469     -0.7637685331     -1.2108095181
 C8       -1.3970097962     -1.2505024504      0.3427308504
 N2       -0.5098040126      0.3384788708      1.9937854999
 C9       -0.7809355634     -0.9765945483      1.7048157628
 C10       0.0083396287      0.6566971508      3.3163660524
 O1       -0.5789335304     -1.8502341960      2.5001359852
 C23      -1.3852657685     -2.7422724180      0.0241824476
 C18       3.1404148198     -1.5854237388     -2.0939425258
 C19       0.7611089937     -1.4794590906     -2.3943597503
 C20       1.7589434982     -0.4566431409     -0.4808693049
 C21       3.0081789542     -0.8665521987     -0.9157180876
 C22       2.0107816632     -1.8884398146     -2.8346390249
 H2       -0.1091270565     -1.7227541450     -2.9806379214
 H5        1.6827206767      0.1098192276      0.4280427660
 H7        3.8794050477     -0.6204806029     -0.3342727882
 H8        2.0981865684     -2.4407343996     -3.7542895653
 H9        4.1121430887     -1.9008311425     -2.4311357817
 H10      -1.4333317032     -0.4538725069     -1.6215498898
 H19      -0.3751247902     -3.1286472974     -0.0211710045
 H20      -1.8644863918     -2.9205929678     -0.9339427550
 H21      -1.9188688753     -3.2942339980      0.7862226037
 H22      -2.4343333792     -0.9275445183      0.4408235038
 H11       0.8106521702      1.3794743443      3.2303002823
 H12       0.3845231136     -0.2494763252      3.7579642006
 H13      -0.7660019670      1.0631393006      3.9596008050

 nuclear repulsion energy.......  1414.901765060 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  32   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.333E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom         H1     C1      C2      C3      C4      C5      C6
C7
  grid # 1        72     87      89      90      89      88      84
81
  grid # 2       116     97      96      98      97      97      94
90
  grid # 3       217    182     184     194     183     184     189
177
  grid # 4       216    326     328     338     328     328     323
314

  number of gridpoints:
     atom         H3     H4      H6     C16      C8      N2      C9
C10
  grid # 1        73     73      70      92      82      95      82
69
  grid # 2       118    118     112     100      90     105      92
78
  grid # 3       223    223     207     194     174     211     176
147
  grid # 4       224    223     207     342     311     387     293
275

  number of gridpoints:
     atom         O1    C23     C18     C19     C20     C21     C22
H2
  grid # 1       111     74      89      88      88      89      89
71
  grid # 2       123     80      97      95      96      97      96
112
  grid # 3       257    150     183     183     182     184     183
212
  grid # 4       450    286     327     326     327     327     327
211

  number of gridpoints:
     atom         H5     H7      H8      H9     H10     H19     H20
H21
  grid # 1        71     73      73      73      67      71      71
70
  grid # 2       111    118     118     118     106     108     110
108
  grid # 3       212    223     223     224     202     218     216
217
  grid # 4       207    223     224     224     197     212     216
215

  number of gridpoints:
     atom        H22    H11     H12     H13  total
```

```
  grid # 1       69     71     70     71   2865
  grid # 2      110    109    107    111   3728
  grid # 3      214    214    212    217   7191
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  1  U  -783.03314743173           2.4E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03324478760  9.7E-05   1.1E-05  5.1E-04
etot  3  Y  Y  4  M  -783.03326229853  1.8E-05   3.6E-06  1.3E-04
etot  4  Y  N  4  M  -783.03326106824 -1.2E-06   0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.90176505953
   (E)  Total one-electron terms..... -3874.37697560531
   (I)  Total two-electron terms.....  1676.44194947754
   (L)  Electronic energy............. -2197.93502612777  (E+I)
   (N)  Total energy.................  -783.03326106824  (A+L)

 SCFE: SCF energy: HF    -783.03326106824 hartrees   iterations:
4


 HOMO energy:    -0.30202
 LUMO energy:     0.12927

  Orbital energies:
  -20.52694  -15.60012  -11.34584  -11.28575  -11.25658  -11.24981
  -11.24298  -11.24133  -11.24050  -11.23870  -11.23789  -11.23490
  -11.23148  -11.23060  -11.23015  -11.22981  -11.22869  -11.22759
  -11.20918   -1.39747   -1.26945   -1.16500   -1.14893   -1.10596
   -1.03001   -1.01861   -1.01780   -1.01269   -0.96256   -0.93266
   -0.85808   -0.83890   -0.83325   -0.82165   -0.79604   -0.74108
   -0.71095   -0.69497   -0.67283   -0.66426   -0.64456   -0.63754
   -0.62742   -0.61486   -0.61224   -0.60849   -0.59695   -0.58335
   -0.57625   -0.55335   -0.54871   -0.54064   -0.53101   -0.51902
   -0.51488   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
   -0.46284   -0.42151   -0.41150   -0.34254   -0.33294   -0.32284
   -0.30202    0.12927    0.13402    0.14450    0.15237    0.20398
```

0.22970 0.24104 0.24880 0.26135 0.28823

end of program scf

start of program der1a
end of program der1a

start of program rwr
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	-1.419761E-05	1.695766E-05	3.451910E-05
2	C1	-3.367334E-05	9.312170E-05	-8.954056E-05
3	C2	-6.942521E-05	1.548285E-04	3.166290E-05
4	C3	-2.689030E-05	-9.322543E-06	-2.003455E-04
5	C4	-1.968315E-05	8.996926E-05	4.508059E-05
6	C5	-2.707885E-05	5.976129E-05	-2.061409E-05
7	C6	8.972692E-05	3.456596E-06	1.488584E-04
8	C7	-1.299157E-04	-4.857736E-05	-6.538914E-05
9	H3	2.345681E-06	-3.370563E-05	5.270973E-05
10	H4	-5.421775E-06	-3.746798E-05	-1.234728E-05
11	H6	-3.521005E-05	3.644945E-05	-6.042547E-05
12	C16	-3.388753E-05	-2.351240E-04	-8.233923E-05
13	C8	1.571356E-04	9.550692E-05	2.629882E-05
14	N2	-9.565829E-05	3.705487E-04	-3.808719E-04
15	C9	-8.838899E-05	5.709793E-05	1.859701E-04
16	C10	1.319897E-05	1.551264E-04	-2.661046E-05
17	O1	9.299827E-06	-2.350596E-04	1.083959E-04
18	C23	2.499740E-05	-2.396197E-05	4.156761E-07
19	C18	-1.417986E-04	4.402736E-05	-4.853944E-05
20	C19	-9.254293E-05	8.478585E-05	1.110945E-05
21	C20	-6.511603E-05	-2.494568E-04	-3.471868E-04
22	C21	-1.184292E-04	-3.648033E-05	-2.291644E-04
23	C22	6.673478E-05	1.812937E-05	3.627456E-05
24	H2	1.674945E-04	1.144597E-04	1.803355E-04
25	H5	-3.632956E-05	3.075275E-04	1.983242E-04
26	H7	4.576618E-05	7.346262E-05	1.096941E-05
27	H8	-1.239831E-05	8.456940E-05	1.749936E-04
28	H9	-3.424412E-05	5.980291E-05	1.512730E-05
29	H10	3.923015E-05	6.234296E-05	2.264811E-05
30	H19	-1.023405E-04	8.702372E-05	1.992197E-06
31	H20	-4.233409E-05	1.858463E-05	1.620934E-05
32	H21	2.920042E-05	6.727809E-05	-9.444831E-05
33	H22	-4.511039E-05	4.599512E-05	-4.536785E-06

```
 34    H11    -1.626549E-04  -2.943504E-05  -1.333052E-05
 35    H12    -1.248121E-05  -1.386197E-04   5.964935E-05
 36    H13     5.956919E-05  -1.651496E-05   2.440085E-05
-----------   ------------  ------------  ------------
   total      -7.405110E-04   1.107088E-03  -2.897448E-04

 end of program der1b


 start of program geopt  33

 geometry optimization step 33
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0101401
  Cos(theta):   0.7026930

  Final level shift:  -5.8161064E-02

 energy change:          -1.2474E-05 *  (  5.0000E-05 )
 gradient maximum:        7.8846E-04 .  (  4.5000E-04 )
 gradient rms:            1.5754E-04 *  (  3.0000E-04 )
 step size:   0.01014  trust radius:   0.01000
 displacement maximum:    5.9000E-03 .  (  1.8000E-03 )
 displacement rms:        9.1804E-04 *  (  1.2000E-03 )
 predicted energy change:    -9.1894E-06    geom step:   1.0140E-
02    full step:   1.0140E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:     1.2317E-04     y:    -3.6068E-04     z:    -2.5327E-05

 new geometry:
                                 angstroms
 atom            x                   y                   z
 H1       -1.1782436348       1.8884882357     -2.2323451060
 C1       -1.0966500432       2.1210246722     -1.1841919981
 C2       -0.8833985818       2.6953330377      1.5038908766
 C3       -0.8782725170       1.0869161483     -0.2891731885
 C4       -1.2015822621       3.4354136967     -0.7600677729
 C5       -1.0954496818       3.7144926986      0.5900740946
 C6       -0.7673723725       1.3775358407      1.0726829682
 C7       -0.7867648375      -0.3526417995     -0.7565128990
 H3       -1.3664168462       4.2241025129     -1.4717616368
 H4       -1.1816014236       4.7268303196      0.9435337953
 H6       -0.8155656469       2.9335369067      2.5474673153
 C16       0.6129601417      -0.7649483663     -1.2104665821
```

```
  C8       -1.3978387992     -1.2501478148      0.3424335223
  N2       -0.5105536317      0.3377070809      1.9934269523
  C9       -0.7825034468     -0.9774951662      1.7049486950
  C10       0.0060102065      0.6537136930      3.3173250847
  O1       -0.5818155849     -1.8521104528      2.4999057257
  C23      -1.3878093466     -2.7418447005      0.0230860991
  C18       3.1409599414     -1.5829895059     -2.0947304617
  C19       0.7608897374     -1.4866144105     -2.3897620254
  C20       1.7593665998     -0.4490145621     -0.4858643151
  C21       3.0088992520     -0.8569262627     -0.9212972010
  C22       2.0107732232     -1.8945373784     -2.8302508381
  H2       -0.1095125604     -1.7349784475     -2.9723552145
  H5        1.6836957767      0.1261551039      0.4185682141
  H7        3.8809000983     -0.6032399005     -0.3439281192
  H8        2.0979783144     -2.4523120306     -3.7460499885
  H9        4.1131193410     -1.8967451165     -2.4321396604
  H10      -1.4329299787     -0.4533019576     -1.6221184022
  H19      -0.3781689111     -3.1285779634     -0.0242926741
  H20      -1.8692492418     -2.9196334061     -0.9340145266
  H21      -1.9201847187     -3.2937593144      0.7856760704
  H22      -2.4349850328     -0.9262141476      0.4403125226
  H11       0.8084925096      1.3759796254      3.2334841207
  H12       0.3806322747     -0.2541246848      3.7579995218
  H13      -0.7685989033      1.0591796755      3.9608380596

  nuclear repulsion energy.......  1414.898954119 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  33   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
```

```
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
80
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
272

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3730
  grid # 3      214    214    212    217   7188
  grid # 4      211    211    209    218   9912

  end of program grid


  start of program rwr
```

```
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                        RMS     maximum
      e  d  i  u  i                        energy  density   DIIS
      r  t  s  t  d     total energy       change  change    error

etot  1  N  N  1  U  -783.03313364975                2.4E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03323204023  9.8E-05  1.2E-05  5.3E-04
etot  3  Y  Y  4  M  -783.03324395883  1.2E-05  3.6E-06  1.3E-04
etot  4  Y  N  4  M  -783.03324822713  4.3E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89895411906
   (E)  Total one-electron terms..... -3874.36278585393
   (I)  Total two-electron terms.....  1676.43058350774
   (L)  Electronic energy............. -2197.93220234619  (E+I)
   (N)  Total energy.................  -783.03324822713  (A+L)

 SCFE: SCF energy: HF    -783.03324822713 hartrees   iterations:
4


 HOMO energy:    -0.30209
 LUMO energy:     0.12928

  Orbital energies:
  -20.52665  -15.60059  -11.34619  -11.28620  -11.25659  -11.25008
  -11.24314  -11.24173  -11.24053  -11.23854  -11.23794  -11.23493
  -11.23119  -11.23054  -11.22999  -11.22952  -11.22850  -11.22780
  -11.20907   -1.39733   -1.26971   -1.16517   -1.14902   -1.10608
   -1.03012   -1.01870   -1.01795   -1.01270   -0.96258   -0.93279
   -0.85823   -0.83901   -0.83337   -0.82171   -0.79613   -0.74121
   -0.71101   -0.69502   -0.67288   -0.66435   -0.64466   -0.63757
   -0.62743   -0.61492   -0.61226   -0.60861   -0.59695   -0.58330
   -0.57638   -0.55343   -0.54884   -0.54069   -0.53099   -0.51904
   -0.51483   -0.50724   -0.50110   -0.49778   -0.48458   -0.46869
   -0.46290   -0.42165   -0.41156   -0.34266   -0.33292   -0.32296
   -0.30209    0.12928    0.13405    0.14444    0.15224    0.20385
    0.22974    0.24097    0.24890    0.26128    0.28805

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.495729E-05	4.796164E-05	-5.539829E-05
2	C1	-1.014348E-05	-2.750341E-05	6.739713E-05
3	C2	-2.822060E-05	-9.738500E-05	-4.018127E-05
4	C3	2.284691E-05	5.932017E-05	1.836120E-04
5	C4	-2.300864E-05	-2.274707E-05	-6.442334E-05
6	C5	-1.142390E-05	1.248055E-05	6.632482E-06
7	C6	-5.277570E-05	7.152988E-05	-2.027990E-04
8	C7	4.883983E-05	1.062756E-04	4.918108E-05
9	H3	-4.437550E-05	1.003283E-04	-7.334871E-05
10	H4	-3.570224E-05	9.976299E-05	-5.694263E-06
11	H6	-1.690824E-05	3.067899E-05	4.265910E-05
12	C16	-3.563945E-05	3.068864E-04	9.686457E-05
13	C8	-1.493483E-04	-3.820148E-05	-4.727248E-05
14	N2	-1.044950E-05	-3.484935E-04	2.902911E-04
15	C9	-1.096265E-05	3.648476E-05	-1.533171E-04
16	C10	-2.809214E-05	-2.069314E-04	8.277370E-05
17	O1	-4.188463E-05	3.388775E-04	-1.083106E-04
18	C23	-5.089082E-05	7.553558E-05	-3.408758E-05
19	C18	1.384814E-04	1.063206E-05	2.476322E-05
20	C19	5.471999E-05	-3.752327E-05	-5.097231E-05
21	C20	2.837294E-05	3.360736E-04	3.790007E-04
22	C21	9.445389E-05	1.225381E-04	2.480095E-04
23	C22	-1.371408E-04	3.722128E-05	-6.151656E-05
24	H2	-2.254244E-04	-5.388627E-05	-2.202388E-04
25	H5	-1.008995E-06	-2.594671E-04	-2.257091E-04
26	H7	-8.115341E-05	-2.347967E-05	-1.168593E-05
27	H8	-2.847789E-05	-4.385286E-05	-2.322022E-04
28	H9	-7.358682E-06	-4.126945E-06	-3.475342E-05
29	H10	-7.459626E-05	-4.219164E-06	-4.324826E-05
30	H19	3.494792E-05	-2.003829E-05	-7.533938E-06
31	H20	-5.706744E-06	3.578239E-05	-3.419139E-05
32	H21	-7.072750E-05	-8.283587E-06	6.494118E-05
33	H22	-5.694953E-06	6.106126E-06	-1.154229E-05
34	H11	7.608723E-05	1.312416E-04	4.626715E-06
35	H12	-1.280180E-05	2.116719E-04	-7.210344E-05
36	H13	-3.308102E-05	5.136898E-05	-3.433403E-05
total		-7.592054E-04	1.032619E-03	-2.841118E-04

```
 end of program der1b
```

```
  start of program geopt  34

  geometry optimization step 34
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0102892
   Cos(theta):   0.7360524

   Final level shift:  -6.9004093E-02

  energy change:           1.2841E-05 *  (  5.0000E-05 )
  gradient maximum:        8.4139E-04 .  (  4.5000E-04 )
  gradient rms:            1.6553E-04 *  (  3.0000E-04 )
  step size:   0.01029  trust radius:   0.01000
  displacement maximum:    5.8536E-03 .  (  1.8000E-03 )
  displacement rms:        9.3154E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0576E-05    geom step:   1.0289E-
02    full step:   1.0289E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.4661E-04     y:     4.2068E-04     z:     2.7475E-05

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1805614724     1.8873312194    -2.2325590772
  C1       -1.0988678230     2.1203754895    -1.1844499827
  C2       -0.8851972573     2.6958179147     1.5030850454
  C3       -0.8789621666     1.0869655809    -0.2889858675
  C4       -1.2051956092     3.4348036456    -0.7611187766
  C5       -1.0987990691     3.7144821370     0.5889396779
  C6       -0.7679575738     1.3780267725     1.0724270332
  C7       -0.7864899045    -0.3523534833    -0.7563566201
  H3       -1.3713798781     4.2230655574    -1.4732268474
  H4       -1.1860979322     4.7269955359     0.9419277801
  H6       -0.8171292512     2.9343469533     2.5466757310
  C16       0.6132500135    -0.7637463060    -1.2108040406
  C8       -1.3969960689    -1.2503528553     0.3426095063
  N2       -0.5095650235     0.3385205610     1.9935740541
  C9       -0.7810175831    -0.9764387523     1.7047405066
  C10       0.0089396651     0.6565354898     3.3161259514
  O1       -0.5791703716    -1.8499870432     2.5001677177
  C23      -1.3853410052    -2.7421129071     0.0240518728
  C18       3.1404515581    -1.5858894563    -2.0936464290
  C19       0.7612228580    -1.4795130802    -2.3943323359
  C20       1.7590525571    -0.4567842023    -0.4807317457
```

```
  C21       3.0082515555     -0.8669505366     -0.9154375403
  C22       2.0108416635     -1.8887176892     -2.8344753259
  H2       -0.1090067848     -1.7227052760     -2.9806890284
  H5        1.6828091068      0.1096766451      0.4281689213
  H7        3.8794507410     -0.6210694384     -0.3338905403
  H8        2.0982411052     -2.4410615463     -3.7541220756
  H9        4.1121371960     -1.9015237343     -2.4307372788
  H10      -1.4331651322     -0.4537161157     -1.6216716808
  H19      -0.3752573750     -3.1285094964     -0.0212229022
  H20      -1.8645467793     -2.9204454136     -0.9340776715
  H21      -1.9189925001     -3.2940347299      0.7860361960
  H22      -2.4343022302     -0.9273733424      0.4406108339
  H11       0.8103358295      1.3803317714      3.2300391455
  H12       0.3864269001     -0.2494532846      3.7569848015
  H13      -0.7654095882      1.0617010943      3.9601786322

  nuclear repulsion energy.......  1414.901290286 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  34   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.333E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
```

```
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
147
  grid # 4      224    223    208    342    311    387    293
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2865
  grid # 2      110    109    107    111   3728
  grid # 3      214    213    212    217   7190
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
```

```
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -783.03313917140           2.4E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03324190096  1.0E-04  1.2E-05  5.2E-04
etot   3  Y  Y  4  M  -783.03325938365  1.7E-05  3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03325752465 -1.9E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.90129028610
   (E)  Total one-electron terms..... -3874.37617085487
   (I)  Total two-electron terms.....  1676.44162304412
   (L)  Electronic energy............. -2197.93454781075  (E+I)
   (N)  Total energy.................  -783.03325752465  (A+L)

 SCFE: SCF energy: HF    -783.03325752465 hartrees   iterations:
4


 HOMO energy:    -0.30202
 LUMO energy:     0.12927

  Orbital energies:
  -20.52693  -15.60011  -11.34581  -11.28575  -11.25659  -11.24981
  -11.24297  -11.24133  -11.24051  -11.23871  -11.23789  -11.23492
  -11.23148  -11.23061  -11.23015  -11.22982  -11.22869  -11.22759
  -11.20917   -1.39748   -1.26945   -1.16499   -1.14892   -1.10596
   -1.03001   -1.01861   -1.01779   -1.01270   -0.96255   -0.93266
   -0.85808   -0.83890   -0.83325   -0.82165   -0.79604   -0.74108
   -0.71094   -0.69497   -0.67282   -0.66427   -0.64457   -0.63753
   -0.62742   -0.61486   -0.61224   -0.60848   -0.59693   -0.58335
   -0.57625   -0.55335   -0.54872   -0.54064   -0.53100   -0.51903
   -0.51488   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
   -0.46284   -0.42150   -0.41150   -0.34254   -0.33295   -0.32283
   -0.30202    0.12927    0.13402    0.14451    0.15236    0.20399
    0.22969    0.24104    0.24882    0.26136    0.28824

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.423554E-05	1.608411E-05	3.525702E-05
2	C1	-3.217379E-05	9.999231E-05	-8.585930E-05
3	C2	-6.165249E-05	1.450516E-04	2.379150E-05
4	C3	-3.232398E-05	3.252565E-06	-2.059562E-04
5	C4	-1.982986E-05	7.757018E-05	4.177575E-05
6	C5	-2.401762E-05	5.121752E-05	-1.632526E-05
7	C6	6.934168E-05	2.547957E-05	1.511136E-04
8	C7	-1.193000E-04	-5.585110E-05	-6.139549E-05
9	H3	4.042694E-06	-3.701933E-05	5.560441E-05
10	H4	-4.406349E-06	-4.012031E-05	-1.180135E-05
11	H6	-3.448831E-05	3.362757E-05	-6.180295E-05
12	C16	-2.270240E-05	-2.428404E-04	-8.249696E-05
13	C8	1.456418E-04	1.015977E-04	2.288894E-05
14	N2	-7.562233E-05	4.337052E-04	-3.136797E-04
15	C9	-8.327761E-05	3.870506E-05	1.393446E-04
16	C10	1.436637E-05	1.806140E-04	-3.739062E-05
17	O1	3.615547E-06	-2.895078E-04	1.321108E-04
18	C23	1.483506E-05	-8.612687E-06	-6.678258E-06
19	C18	-1.435223E-04	4.785366E-05	-4.370909E-05
20	C19	-1.185819E-04	9.742135E-05	2.455594E-05
21	C20	-8.599774E-05	-2.620429E-04	-3.687782E-04
22	C21	-1.261466E-04	-4.977726E-05	-2.511777E-04
23	C22	9.045403E-05	1.023138E-05	3.016389E-05
24	H2	1.739613E-04	1.186778E-04	1.882769E-04
25	H5	-3.505052E-05	3.124855E-04	2.015493E-04
26	H7	5.350544E-05	7.676913E-05	1.114692E-05
27	H8	-1.161231E-05	9.171525E-05	1.897417E-04
28	H9	-2.986114E-05	6.232830E-05	1.648711E-05
29	H10	3.785039E-05	6.312826E-05	1.889092E-05
30	H19	-7.055307E-05	7.036212E-05	-3.577840E-06
31	H20	-3.775849E-05	2.428104E-05	1.359077E-05
32	H21	1.569277E-05	5.702694E-05	-7.263156E-05
33	H22	-5.728326E-05	5.400058E-05	-3.263135E-06
34	H11	-1.653324E-04	-4.557818E-05	-2.252669E-05
35	H12	-8.525505E-06	-1.416127E-04	5.653734E-05
36	H13	4.831769E-05	-1.993947E-05	3.455181E-06
total		-7.426307E-04	1.100277E-03	-2.927675E-04

end of program der1b

start of program geopt 35

geometry optimization step 35
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0101577
   Cos(theta):   0.7096922

   Final level shift:  -5.9936046E-02

  energy change:          -9.2975E-06 *  (  5.0000E-05 )
  gradient maximum:        8.2905E-04 .  (  4.5000E-04 )
  gradient rms:            1.6182E-04 *  (  3.0000E-04 )
  step size:   0.01016  trust radius:   0.01000
  displacement maximum:    5.8998E-03 .  (  1.8000E-03 )
  displacement rms:        9.1963E-04 *  (  1.2000E-03 )
  predicted energy change:    -9.5346E-06    geom step:   1.0158E-
02    full step:   1.0158E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     4.0183E-05     y:    -4.0817E-04     z:     1.8648E-05

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1780959865     1.8886365093    -2.2324111974
  C1       -1.0965950393     2.1211242707    -1.1842400163
  C2       -0.8836885591     2.6953109023     1.5039080142
  C3       -0.8781839324     1.0870015221    -0.2892482658
  C4       -1.2016859866     3.4354723985    -0.7600460694
  C5       -1.0957554189     3.7144938471     0.5901273141
  C6       -0.7673801867     1.3775867398     1.0726182992
  C7       -0.7866773992    -0.3525701990    -0.7565731427
  H3       -1.3665230583     4.2241851175    -1.4717097388
  H4       -1.1820986030     4.7267978301     0.9436287835
  H6       -0.8160648773     2.9334204885     2.5475241315
  C16       0.6130617601    -0.7649693713    -1.2103997393
  C8       -1.3979711936    -1.2500205454     0.3423146603
  N2       -0.5104319673     0.3377301161     1.9933135921
  C9       -0.7827553530    -0.9774387468     1.7049035016
  C10       0.0067763016     0.6535819869     3.3169727326
  O1       -0.5823909012    -1.8520607931     2.4999656520
  C23      -1.3879911048    -2.7417379021     0.0230017899
  C18       3.1411107946    -1.5831482088    -2.0945005210
  C19       0.7610313221    -1.4867078101    -2.3896467211
  C20       1.7594414390    -0.4490513000    -0.4857668967
  C21       3.0089951627    -0.8570189449    -0.9211192787
  C22       2.0109392888    -1.8947119032    -2.8300487298
  H2       -0.1093420184    -1.7350290935    -2.9722896895
  H5        1.6837650844     0.1261972588     0.4186167921
  H7        3.8809853315    -0.6033099777    -0.3437180405
  H8        2.0981725490    -2.4525322364    -3.7458102377
  H9        4.1132900762    -1.8969284241    -2.4318394277
  H10      -1.4327532368    -0.4531878102    -1.6222577299
```

```
  H19      -0.3783594796     -3.1286260004     -0.0240270515
  H20      -1.8691110612     -2.9194765820     -0.9342678011
  H21      -1.9207117695     -3.2935724368      0.7854473765
  H22      -2.4351208906     -0.9259980847      0.4400534515
  H11       0.8084419856      1.3766802522      3.2327871194
  H12       0.3826692380     -0.2540764040      3.7569549745
  H13      -0.7677554457      1.0579670118      3.9612344789

  nuclear repulsion energy.......  1414.895433378 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  35   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
80
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
272
```

```
  number of gridpoints:
     atom         O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1       111     74     89     88     88     89     89
71
  grid # 2       123     79     97     95     96     97     96
112
  grid # 3       257    149    183    183    182    184    183
212
  grid # 4       450    287    327    326    327    327    327
211

  number of gridpoints:
     atom         H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1        71     73     73     73     66     71     71
70
  grid # 2       111    118    118    118    106    108    110
108
  grid # 3       212    223    223    224    203    218    217
217
  grid # 4       207    223    224    224    196    212    216
215

  number of gridpoints:
     atom        H22    H11    H12    H13  total
  grid # 1        69     71     70     71   2863
  grid # 2       110    109    107    111   3730
  grid # 3       214    213    212    217   7187
  grid # 4       211    211    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03312817429           2.5E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03322983626  1.0E-04  1.2E-05  5.3E-04
etot   3  Y  Y  4  M  -783.03324267598  1.3E-05  3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03324656249  3.9E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
```

```
   (A)  Nuclear repulsion.....  1414.89543337819
   (E)  Total one-electron terms..... -3874.35563247521
   (I)  Total two-electron terms.....  1676.42695253453
   (L)  Electronic energy..... -2197.92867994068  (E+I)
   (N)  Total energy.............  -783.03324656249  (A+L)

 SCFE: SCF energy: HF    -783.03324656249 hartrees   iterations:
4


 HOMO energy:    -0.30209
 LUMO energy:     0.12928

  Orbital energies:
 -20.52664  -15.60059  -11.34619  -11.28620  -11.25659  -11.25009
 -11.24314  -11.24174  -11.24054  -11.23855  -11.23794  -11.23493
 -11.23120  -11.23056  -11.22999  -11.22951  -11.22850  -11.22780
 -11.20908   -1.39731   -1.26971   -1.16517   -1.14902   -1.10608
  -1.03012   -1.01871   -1.01795   -1.01270   -0.96258   -0.93279
  -0.85823   -0.83901   -0.83337   -0.82171   -0.79613   -0.74121
  -0.71101   -0.69502   -0.67287   -0.66435   -0.64466   -0.63757
  -0.62743   -0.61492   -0.61226   -0.60861   -0.59694   -0.58330
  -0.57639   -0.55344   -0.54884   -0.54069   -0.53098   -0.51904
  -0.51483   -0.50724   -0.50111   -0.49778   -0.48458   -0.46869
  -0.46290   -0.42164   -0.41155   -0.34266   -0.33292   -0.32297
  -0.30209    0.12928    0.13405    0.14443    0.15223    0.20385
   0.22972    0.24095    0.24889    0.26128    0.28804

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x             y             z
 ----  -----   -------------  -------------  -------------
   1    H1     -2.535610E-05   4.765911E-05  -5.461188E-05
   2    C1     -9.566438E-06  -3.364197E-05   6.620546E-05
   3    C2     -2.159057E-05  -8.669955E-05  -3.389464E-05
   4    C3      2.544861E-05   5.198787E-05   1.829793E-04
   5    C4     -2.354193E-05  -1.746254E-05  -6.225811E-05
   6    C5     -1.197278E-05   1.844462E-05   6.462218E-06
   7    C6     -4.894027E-05   5.798080E-05  -2.025740E-04
```

```
 8    C7      4.445640E-05   1.087713E-04   4.496167E-05
 9    H3     -4.579615E-05   1.010771E-04  -7.304683E-05
10    H4     -3.682852E-05   1.021405E-04  -4.473549E-06
11    H6     -1.684824E-05   3.192090E-05   4.313067E-05
12    C16    -3.628948E-05   3.001228E-04   9.402457E-05
13    C8     -1.492883E-04  -4.602869E-05  -3.773039E-05
14    N2     -1.978983E-05  -3.910021E-04   2.563304E-04
15    C9     -2.370911E-06   3.841507E-05  -1.301884E-04
16    C10    -3.396275E-05  -2.068337E-04   7.879877E-05
17    O1     -4.035825E-05   3.770991E-04  -1.322296E-04
18    C23    -4.845145E-05   6.976128E-05  -2.505076E-05
19    C18     1.284974E-04   9.151605E-06   2.561810E-05
20    C19     7.780482E-05  -4.045839E-05  -5.560339E-05
21    C20     4.424364E-05   3.427295E-04   3.820855E-04
22    C21     9.727075E-05   1.256628E-04   2.558036E-04
23    C22    -1.494975E-04   4.572891E-05  -5.479044E-05
24    H2     -2.279007E-04  -5.747398E-05  -2.233183E-04
25    H5     -1.789975E-06  -2.624105E-04  -2.270184E-04
26    H7     -9.041280E-05  -2.700797E-05  -1.513422E-05
27    H8     -2.928528E-05  -4.576682E-05  -2.358365E-04
28    H9     -1.124274E-05  -5.693067E-06  -3.468369E-05
29    H10    -7.297373E-05  -3.909792E-06  -3.925837E-05
30    H19     1.741090E-05  -1.032409E-05  -8.510606E-06
31    H20    -1.023351E-05   3.199483E-05  -3.258801E-05
32    H21    -5.905993E-05  -2.102603E-07   4.849995E-05
33    H22     5.346530E-06  -2.507314E-07  -1.420271E-05
34    H11     8.647774E-05   1.372383E-04   1.131339E-05
35    H12    -1.819118E-05   2.089626E-04  -6.810475E-05
36    H13    -3.464694E-05   5.704635E-05  -1.799398E-05
-----------   -------------  -------------  -------------
  total      -7.492295E-04   1.028721E-03  -2.868879E-04

 end of program der1b


 start of program geopt  36

 geometry optimization step 36
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0102835
  Cos(theta):   0.7341947

  Final level shift:  -6.8733468E-02

 energy change:           1.0962E-05 *  (  5.0000E-05 )
 gradient maximum:        8.6702E-04 .  (  4.5000E-04 )
```

```
  gradient rms:            1.6867E-04 *  (  3.0000E-04 )
  step size:   0.01028  trust radius:   0.01000
  displacement maximum:    5.8925E-03 .  (  1.8000E-03 )
  displacement rms:        9.3103E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0667E-05    geom step:   1.0284E-
02    full step:   1.0284E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -6.4925E-05     y:     4.4896E-04     z:    -5.3046E-06

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1805528852     1.8875051559    -2.2325992874
  C1       -1.0989035971     2.1205019756    -1.1844759532
  C2       -0.8854915894     2.6958546792     1.5031139859
  C3       -0.8788426726     1.0870766430    -0.2890592261
  C4       -1.2054736696     3.4348986971    -0.7610703803
  C5       -1.0992376625     3.7145377338     0.5890140734
  C6       -0.7678963520     1.3781164489     1.0723596808
  C7       -0.7863737720    -0.3522496785    -0.7564254353
  H3       -1.3717811057     4.2231693968    -1.4731444044
  H4       -1.1868089968     4.7270146736     0.9420497937
  H6       -0.8176257101     2.9343036896     2.5467414165
  C16       0.6133623923    -0.7637564241    -1.2107874648
  C8       -1.3969896918    -1.2502314714     0.3425143560
  N2       -0.5093971497     0.3385732380     1.9934338244
  C9       -0.7811022844    -0.9763194272     1.7046850964
  C10       0.0094443589     0.6564384979     3.3159279632
  O1       -0.5794224150    -1.8498062899     2.5002037102
  C23      -1.3854115319    -2.7419786793     0.0239218948
  C18       3.1404962580    -1.5862662863    -2.0934242909
  C19       0.7613255769    -1.4795609208    -2.3943070261
  C20       1.7591553638    -0.4569244010    -0.4806250737
  C21       3.0083222558    -0.8672893347    -0.9152264890
  C22       2.0109043909    -1.8889377589    -2.8343547660
  H2       -0.1088969944    -1.7226515331    -2.9807293551
  H5        1.6829092815     0.1095511988     0.4282625539
  H7        3.8795027701    -0.6215599304    -0.3336006551
  H8        2.0982996338    -2.4413024832    -3.7540017213
  H9        4.1121535243    -1.9020638276    -2.4304368222
  H10      -1.4330103024    -0.4535887687    -1.6217671664
  H19      -0.3753680097    -3.1284214900    -0.0213323770
  H20      -1.8646329951    -2.9202988912    -0.9342018880
  H21      -1.9190862659    -3.2938801425     0.7858722684
  H22      -2.4342889348    -0.9272273551     0.4404252245
  H11       0.8100960870     1.3810484584     3.2297678723
  H12       0.3880011928    -0.2493939840     3.7561937750
  H13      -0.7649047806     1.0605791291     3.9606357410

  nuclear repulsion energy.......  1414.897598326 hartrees
```

```
  ------------------------------------------------
 /  end of geometry optimization iteration  36   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.334E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
147
  grid # 4      224    223    208    342    311    387    293
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
```

```
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2864
  grid # 2      110    109    107    111   3728
  grid # 3      214    213    212    217   7190
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                          RMS    maximum
      t  p  i  c  r                              energy  density   DIIS
      e  d  i  u  i                              change  change    error
      r  t  s  t  d     total energy

etot  1  N  N  1  U  -783.03313608647                    2.5E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03324063193  1.0E-04  1.2E-05  5.3E-04
etot  3  Y  Y  4  M  -783.03325820681  1.8E-05  3.7E-06  1.3E-04
etot  4  Y  N  4  M  -783.03325709643 -1.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89759832643
   (E)  Total one-electron terms..... -3874.36886240210
   (I)  Total two-electron terms.....  1676.43800697924
   (L)  Electronic energy............. -2197.93085542286  (E+I)
   (N)  Total energy.................  -783.03325709643  (A+L)

 SCFE: SCF energy: HF    -783.03325709643 hartrees   iterations:
4
```

```
HOMO energy:    -0.30203
LUMO energy:     0.12928

 Orbital energies:
 -20.52693  -15.60010  -11.34580  -11.28575  -11.25659  -11.24981
 -11.24296  -11.24133  -11.24051  -11.23871  -11.23790  -11.23492
 -11.23148  -11.23061  -11.23016  -11.22982  -11.22870  -11.22760
 -11.20917   -1.39749   -1.26944   -1.16499   -1.14892   -1.10595
  -1.03001   -1.01861   -1.01779   -1.01270   -0.96255   -0.93266
  -0.85808   -0.83890   -0.83325   -0.82165   -0.79604   -0.74108
  -0.71094   -0.69497   -0.67282   -0.66427   -0.64457   -0.63753
  -0.62742   -0.61486   -0.61224   -0.60848   -0.59692   -0.58336
  -0.57625   -0.55336   -0.54872   -0.54064   -0.53099   -0.51904
  -0.51488   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
  -0.46284   -0.42149   -0.41149   -0.34254   -0.33295   -0.32283
  -0.30203    0.12928    0.13402    0.14451    0.15236    0.20400
   0.22969    0.24104    0.24883    0.26136    0.28825

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -1.421422E-05   1.622406E-05   3.560901E-05
  2    C1     -3.080083E-05   1.051433E-04  -8.263252E-05
  3    C2     -5.691957E-05   1.383546E-04   1.688220E-05
  4    C3     -3.691211E-05   1.051349E-05  -2.069443E-04
  5    C4     -1.969678E-05   7.274869E-05   4.063217E-05
  6    C5     -2.273164E-05   4.388447E-05  -1.617513E-05
  7    C6      5.562941E-05   3.228462E-05   1.572859E-04
  8    C7     -1.121306E-04  -5.746059E-05  -5.729849E-05
  9    H3      5.409488E-06  -3.934592E-05   5.634476E-05
 10    H4     -3.212848E-06  -4.309686E-05  -1.262733E-05
 11    H6     -3.317529E-05   3.122733E-05  -6.182656E-05
 12    C16    -1.860782E-05  -2.420060E-04  -8.275357E-05
 13    C8      1.366346E-04   1.090754E-04   1.336622E-05
 14    N2     -6.348470E-05   4.613149E-04  -2.851330E-04
 15    C9     -7.796635E-05   3.691730E-05   1.210489E-04
 16    C10     1.208864E-05   1.943362E-04  -4.546085E-05
```

```
 17    O1      2.410879E-06  -3.193304E-04   1.445500E-04
 18    C23     1.314074E-05  -4.061377E-06  -7.661916E-06
 19    C18    -1.422226E-04   4.938421E-05  -4.158892E-05
 20    C19    -1.343307E-04   1.043663E-04   3.187558E-05
 21    C20    -9.955109E-05  -2.681346E-04  -3.782832E-04
 22    C21    -1.296386E-04  -5.621549E-05  -2.617739E-04
 23    C22     1.045027E-04   6.905157E-06   2.768787E-05
 24    H2      1.767673E-04   1.205974E-04   1.926198E-04
 25    H5     -3.470847E-05   3.133744E-04   2.023798E-04
 26    H7      5.895365E-05   7.926851E-05   1.130112E-05
 27    H8     -1.136032E-05   9.520055E-05   1.968011E-04
 28    H9     -2.719035E-05   6.329673E-05   1.684234E-05
 29    H10     3.727970E-05   6.371943E-05   1.676385E-05
 30    H19    -5.594514E-05   6.409139E-05  -6.530179E-06
 31    H20    -3.464908E-05   2.867019E-05   1.189737E-05
 32    H21     6.671015E-06   5.012837E-05  -5.851659E-05
 33    H22    -6.214990E-05   5.878777E-05  -1.602531E-06
 34    H11    -1.652207E-04  -5.559288E-05  -2.654897E-05
 35    H12    -6.523428E-06  -1.432918E-04   5.447587E-05
 36    H13     4.117845E-05  -2.060084E-05  -7.638846E-06
-----------   -------------  -------------  -------------
   total      -7.426767E-04   1.100678E-03  -2.926329E-04

 end of program der1b


 start of program geopt  37

 geometry optimization step 37
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0101675
  Cos(theta):   0.7121716

  Final level shift:  -6.0789028E-02

 energy change:          -1.0534E-05 *  (  5.0000E-05 )
 gradient maximum:        8.4714E-04 .  (  4.5000E-04 )
 gradient rms:            1.6444E-04 *  (  3.0000E-04 )
 step size:   0.01017  trust radius:   0.01000
 displacement maximum:    5.8939E-03 .  (  1.8000E-03 )
 displacement rms:        9.2052E-04 *  (  1.2000E-03 )
 predicted energy change:    -9.7181E-06    geom step:   1.0168E-
02    full step:   1.0168E-02
 molecular structure not yet converged...

 center of mass moved by:
```

```
   x:    -1.4503E-06     y:    -4.3085E-04     z:     3.4521E-05

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1780098894     1.8887544911    -2.2324632597
 C1       -1.0965697255     2.1212064206    -1.1842792882
 C2       -0.8839258530     2.6953083894     1.5039143541
 C3       -0.8781020208     1.0870775179    -0.2893102970
 C4       -1.2018132568     3.4355207527    -0.7600344969
 C5       -1.0960350414     3.7145024050     0.5901606857
 C6       -0.7673708777     1.3776404944     1.0725627615
 C7       -0.7866030439    -0.3525052219    -0.7566207331
 H3       -1.3666861238     4.2242417020    -1.4716772916
 H4       -1.1825553221     4.7267785049     0.9436906374
 H6       -0.8164765755     2.9333469055     2.5475617363
 C16       0.6131417686    -0.7649859386    -1.2103527003
 C8       -1.3980510463    -1.2499147580     0.3422266831
 N2       -0.5103221891     0.3377601966     1.9932154100
 C9       -0.7829181526    -0.9773740956     1.7048669668
 C10       0.0073420459     0.6534770624     3.3167211228
 O1       -0.5827735928    -1.8519884375     2.5000116490
 C23      -1.3881191576    -2.7416442728     0.0229384326
 C18       3.1412136689    -1.5833246169    -2.0943125378
 C19       0.7611369782    -1.4867493291    -2.3895828406
 C20       1.7595013156    -0.4491307393    -0.4856723298
 C21       3.0090640036    -0.8571738142    -0.9209505771
 C22       2.0110563471    -1.8948360931    -2.8299138852
 H2       -0.1092159932    -1.7350094455    -2.9722805179
 H5        1.6838238496     0.1261446981     0.4186911658
 H7        3.8810433554    -0.6035007790    -0.3434999542
 H8        2.0983062971    -2.4526652744    -3.7456670137
 H9        4.1134004863    -1.8971526739    -2.4315923249
 H10      -1.4326137959    -0.4530906697    -1.6223606981
 H19      -0.3785007452    -3.1286324123    -0.0239116735
 H20      -1.8690820406    -2.9193517764    -0.9344147207
 H21      -1.9210268019    -3.2934262614     0.7853148752
 H22      -2.4352007591    -0.9258313967     0.4398668595
 H11       0.8083480772     1.3772599696     3.2323237922
 H12       0.3842430289    -0.2540387549     3.7561520200
 H13      -0.7671478746     1.0569756258     3.9615737830

 nuclear repulsion energy.......  1414.893099359 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  37   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.335E-04
```

```
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
```

```
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3729
  grid # 3      214    213    212    217   7187
  grid # 4      211    211    209    218   9913

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03312783248           2.5E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03323054953  1.0E-04  1.2E-05  5.4E-04
etot   3  Y  Y  4  M  -783.03324337147  1.3E-05  3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03324718516  3.8E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89309935852
   (E)  Total one-electron terms..... -3874.35101188418
   (I)  Total two-electron terms.....  1676.42466534051
   (L)  Electronic energy............. -2197.92634654368  (E+I)
   (N)  Total energy.................  -783.03324718516  (A+L)

 SCFE: SCF energy: HF    -783.03324718516 hartrees   iterations:
4


 HOMO energy:    -0.30210
 LUMO energy:     0.12929

  Orbital energies:
  -20.52664  -15.60058  -11.34619  -11.28620  -11.25659  -11.25009
  -11.24315  -11.24174  -11.24054  -11.23855  -11.23794  -11.23493
  -11.23120  -11.23055  -11.23000  -11.22953  -11.22851  -11.22780
```

```
-11.20908   -1.39730   -1.26970   -1.16517   -1.14902   -1.10607
 -1.03012   -1.01871   -1.01796   -1.01270   -0.96258   -0.93279
 -0.85823   -0.83901   -0.83337   -0.82172   -0.79613   -0.74121
 -0.71100   -0.69502   -0.67287   -0.66435   -0.64467   -0.63757
 -0.62743   -0.61492   -0.61225   -0.60861   -0.59694   -0.58330
 -0.57639   -0.55345   -0.54884   -0.54068   -0.53097   -0.51904
 -0.51483   -0.50724   -0.50111   -0.49778   -0.48458   -0.46869
 -0.46290   -0.42163   -0.41155   -0.34266   -0.33292   -0.32297
 -0.30210    0.12929    0.13404    0.14443    0.15223    0.20384
  0.22972    0.24095    0.24891    0.26128    0.28802

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
   1    H1     -2.558109E-05   4.764163E-05  -5.461483E-05
   2    C1     -9.694870E-06  -3.621850E-05   6.375362E-05
   3    C2     -1.881120E-05  -8.829173E-05  -2.992817E-05
   4    C3      2.176462E-05   4.881963E-05   1.836421E-04
   5    C4     -2.321922E-05  -1.265752E-05  -5.966461E-05
   6    C5     -1.535243E-05   1.919338E-05  -6.431766E-07
   7    C6     -5.036272E-05   4.182262E-05  -1.969955E-04
   8    C7      4.748481E-05   1.128321E-04   4.001148E-05
   9    H3     -4.651797E-05   1.040032E-04  -7.530917E-05
  10    H4     -3.752926E-05   1.036654E-04  -4.047348E-06
  11    H6     -1.425323E-05   3.041198E-05   4.520956E-05
  12    C16    -3.628711E-05   2.970491E-04   8.982047E-05
  13    C8     -1.507670E-04  -4.732473E-05  -4.208407E-05
  14    N2     -1.947924E-05  -4.196673E-04   2.360812E-04
  15    C9      7.222703E-07   4.566022E-05  -1.083424E-04
  16    C10    -3.707115E-05  -2.045319E-04   7.531876E-05
  17    O1     -3.883083E-05   3.986977E-04  -1.487326E-04
  18    C23    -4.396610E-05   6.162328E-05  -1.864912E-05
  19    C18     1.233810E-04   9.135880E-06   2.498330E-05
  20    C19     9.026617E-05  -4.410007E-05  -6.093035E-05
  21    C20     5.466546E-05   3.445673E-04   3.865912E-04
  22    C21     1.000057E-04   1.293587E-04   2.613709E-04
  23    C22    -1.556441E-04   5.124867E-05  -5.037288E-05
  24    H2     -2.279003E-04  -5.839602E-05  -2.232224E-04
```

```
  25    H5     -3.495610E-06  -2.621306E-04  -2.254230E-04
  26    H7     -9.633620E-05  -2.733072E-05  -1.832394E-05
  27    H8     -2.974756E-05  -4.647492E-05  -2.362929E-04
  28    H9     -1.414532E-05  -6.573289E-06  -3.474903E-05
  29    H10    -7.305411E-05  -4.604335E-06  -3.687351E-05
  30    H19     3.163693E-06  -3.347030E-06  -7.087484E-06
  31    H20    -1.241795E-05   2.993322E-05  -3.257361E-05
  32    H21    -5.362958E-05   4.149991E-06   4.073772E-05
  33    H22     1.212486E-05  -3.275757E-06  -1.418639E-05
  34    H11     9.140831E-05   1.381627E-04   1.499670E-05
  35    H12    -2.299067E-05   2.106471E-04  -6.872140E-05
  36    H13    -3.854167E-05   6.136728E-05  -1.041159E-05
 -----------   -------------  -------------  -------------
    total      -7.506396E-04   1.025066E-03  -2.956625E-04

  end of program der1b


  start of program geopt  38

  geometry optimization step 38
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0102741
   Cos(theta):   0.7327022

   Final level shift:  -6.8279924E-02

  energy change:           9.9113E-06 *  (  5.0000E-05 )
  gradient maximum:        8.6857E-04 .  (  4.5000E-04 )
  gradient rms:            1.6997E-04 *  (  3.0000E-04 )
  step size:   0.01027  trust radius:   0.01000
  displacement maximum:    5.8986E-03 .  (  1.8000E-03 )
  displacement rms:        9.3017E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0670E-05    geom step:   1.0274E-
02    full step:   1.0274E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.0284E-05     y:     4.5568E-04     z:    -2.9104E-05

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1805551294     1.8876302015    -2.2326508487
  C1       -1.0989315220     2.1205852778    -1.1845163662
  C2       -0.8856938977     2.6958388767     1.5031156600
```

```
 C3       -0.8787611130      1.0871462361     -0.2891353249
 C4       -1.2056702049      3.4349537753     -0.7610528278
 C5       -1.0995423743      3.7145402322      0.5890516678
 C6       -0.7678462856      1.3781521188      1.0722920964
 C7       -0.7862987866     -0.3521863950     -0.7564912029
 H3       -1.3720603692      4.2232383701     -1.4730985536
 H4       -1.1872963883      4.7269875023      0.9421293809
 H6       -0.8179502662      2.9342162880      2.5467724565
 C16       0.6134453593     -0.7637691733     -1.2107605799
 C8       -1.3970317927     -1.2501274008      0.3424339158
 N2       -0.5092493934      0.3385897208      1.9933100453
 C9       -0.7811961383     -0.9762340452      1.7046440609
 C10       0.0098942999      0.6563308085      3.3157376699
 O1       -0.5796528777     -1.8496842305      2.5002275168
 C23      -1.3855788918     -2.7418879859      0.0238827379
 C18       3.1405695947     -1.5864626122     -2.0932272572
 C19       0.7614317672     -1.4795883185     -2.3942728769
 C20       1.7592151558     -0.4570053713     -0.4805211010
 C21       3.0083802237     -0.8674658202     -0.9150382568
 C22       2.0110039561     -1.8890524356     -2.8342377321
 H2       -0.1087748604     -1.7226095131     -2.9807535654
 H5        1.6829500067      0.1094863325      0.4283518089
 H7        3.8795410835     -0.6218107255     -0.3333546053
 H8        2.0984151874     -2.4414296767     -3.7538835719
 H9        4.1122179609     -1.9023480267     -2.4301785900
 H10      -1.4328902973     -0.4535128545     -1.6218643806
 H19      -0.3755819445     -3.1284172346     -0.0213222745
 H20      -1.8648032911     -2.9202026190     -0.9342422346
 H21      -1.9193263352     -3.2937162139      0.7858334384
 H22      -2.4343162973     -0.9270580337      0.4402837571
 H11       0.8099398723      1.3815932732      3.2294990387
 H12       0.3893372430     -0.2493722273      3.7555082582
 H13      -0.7644454903      1.0596392912      3.9609788952

 nuclear repulsion energy.......  1414.896952044 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  38   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.334E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
147
  grid # 4      224    223    208    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
```

```
  grid # 1       69     71     70     71   2864
  grid # 2      110    109    108    111   3729
  grid # 3      214    213    212    217   7190
  grid # 4      211    211    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  1  U  -783.03313554497           2.5E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03324073977  1.1E-04   1.2E-05  5.3E-04
etot  3  Y  Y  4  M  -783.03325788170  1.7E-05   3.7E-06  1.3E-04
etot  4  Y  N  4  M  -783.03325660737 -1.3E-06   0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89695204358
   (E)  Total one-electron terms..... -3874.36757926531
   (I)  Total two-electron terms.....  1676.43737061437
   (L)  Electronic energy............. -2197.93020865095  (E+I)
   (N)  Total energy.................  -783.03325660737  (A+L)

 SCFE: SCF energy: HF    -783.03325660737 hartrees   iterations:
4


 HOMO energy:    -0.30203
 LUMO energy:     0.12928

  Orbital energies:
  -20.52692  -15.60009  -11.34579  -11.28574  -11.25660  -11.24981
  -11.24296  -11.24133  -11.24051  -11.23871  -11.23790  -11.23493
  -11.23148  -11.23061  -11.23017  -11.22982  -11.22870  -11.22760
  -11.20917   -1.39749   -1.26944   -1.16499   -1.14892   -1.10595
   -1.03001   -1.01861   -1.01779   -1.01270   -0.96255   -0.93266
   -0.85808   -0.83891   -0.83326   -0.82165   -0.79604   -0.74108
   -0.71094   -0.69497   -0.67281   -0.66427   -0.64458   -0.63752
   -0.62742   -0.61486   -0.61224   -0.60847   -0.59691   -0.58336
   -0.57624   -0.55337   -0.54872   -0.54064   -0.53099   -0.51904
   -0.51487   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
   -0.46284   -0.42149   -0.41149   -0.34253   -0.33295   -0.32283
   -0.30203    0.12928    0.13401    0.14451    0.15236    0.20400
```

```
   0.22969    0.24104    0.24884    0.26136    0.28825

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.398445E-05	1.503832E-05	3.577500E-05
2	C1	-3.017484E-05	1.039840E-04	-8.096924E-05
3	C2	-5.272708E-05	1.437063E-04	1.623343E-05
4	C3	-4.040740E-05	1.207328E-05	-2.076370E-04
5	C4	-1.919358E-05	6.981469E-05	4.044953E-05
6	C5	-2.161912E-05	4.342789E-05	-1.219258E-05
7	C6	4.672040E-05	3.559405E-05	1.566970E-04
8	C7	-1.080201E-04	-6.066380E-05	-5.355723E-05
9	H3	6.215848E-06	-4.136248E-05	5.850796E-05
10	H4	-3.031220E-06	-4.333894E-05	-1.226948E-05
11	H6	-3.411566E-05	3.171966E-05	-6.360408E-05
12	C16	-1.737377E-05	-2.418432E-04	-8.162114E-05
13	C8	1.292981E-04	1.092009E-04	1.907578E-05
14	N2	-5.538742E-05	4.821138E-04	-2.664669E-04
15	C9	-7.234815E-05	2.687622E-05	9.857525E-05
16	C10	1.142167E-05	2.046857E-04	-5.182523E-05
17	O1	-1.841168E-07	-3.379504E-04	1.529862E-04
18	C23	6.786875E-06	1.626234E-06	-8.350499E-06
19	C18	-1.432828E-04	4.939406E-05	-4.136158E-05
20	C19	-1.400756E-04	1.081144E-04	3.601362E-05
21	C20	-1.033761E-04	-2.702268E-04	-3.841537E-04
22	C21	-1.322794E-04	-5.995885E-05	-2.671739E-04
23	C22	1.102365E-04	3.983540E-06	2.515502E-05
24	H2	1.785265E-04	1.204218E-04	1.943111E-04
25	H5	-3.549816E-05	3.133566E-04	2.033529E-04
26	H7	6.004133E-05	8.025631E-05	1.126847E-05
27	H8	-1.048076E-05	9.768682E-05	2.011678E-04
28	H9	-2.544794E-05	6.399926E-05	1.727296E-05
29	H10	3.670387E-05	6.416910E-05	1.500928E-05
30	H19	-4.596635E-05	5.949003E-05	-8.537426E-06
31	H20	-3.242425E-05	2.994185E-05	1.168120E-05
32	H21	6.553888E-06	5.068087E-05	-5.658442E-05
33	H22	-6.213247E-05	6.098173E-05	-2.224601E-06

```
 34    H11    -1.633384E-04  -6.081377E-05  -2.943311E-05
 35    H12    -6.335575E-06  -1.452494E-04   5.406241E-05
 36    H13     3.502740E-05  -2.019874E-05  -1.219174E-05
-----------   -------------  -------------  -------------
   total      -7.416725E-04   1.100731E-03  -2.925588E-04

 end of program der1b


 start of program geopt  39

 geometry optimization step 39
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0101736
  Cos(theta):   0.7136908

  Final level shift:  -6.1301035E-02

 energy change:          -9.4222E-06 *  (  5.0000E-05 )
 gradient maximum:        8.4978E-04 .  (  4.5000E-04 )
 gradient rms:            1.6570E-04 *  (  3.0000E-04 )
 step size:   0.01017  trust radius:   0.01000
 displacement maximum:    5.8860E-03 .  (  1.8000E-03 )
 displacement rms:        9.2108E-04 *  (  1.2000E-03 )
 predicted energy change:    -9.8170E-06    geom step:   1.0174E-
02    full step:   1.0174E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -2.5012E-05     y:    -4.4178E-04     z:     4.9325E-05

 new geometry:
                                 angstroms
 atom            x                  y                  z
 H1       -1.1779593606      1.8888472830     -2.2325084884
 C1       -1.0965641099      2.1212715617     -1.1843146083
 C2       -0.8841244514      2.6953059716      1.5039178010
 C3       -0.8780418791      1.0871363558     -0.2893665598
 C4       -1.2019365270      3.4355603720     -0.7600254941
 C5       -1.0962797517      3.7145108690      0.5901871233
 C6       -0.7673620854      1.3776793269      1.0725117202
 C7       -0.7865442359     -0.3524542322     -0.7566636680
 H3       -1.3668440048      4.2242909592     -1.4716490406
 H4       -1.1829484821      4.7267651607      0.9437422698
 H6       -0.8168103183      2.9332868393      2.5475894156
 C16       0.6132064610     -0.7650003831     -1.2103118614
```

```
  C8       -1.3981102056     -1.2498280704      0.3421556045
  N2       -0.5102145435      0.3377810777      1.9931235428
  C9       -0.7830246481     -0.9773217306      1.7048285324
  C10       0.0078076524      0.6533976879      3.3165115407
  O1       -0.5830429477     -1.8519248740      2.5000363461
  C23      -1.3882443955     -2.7415623093      0.0228822233
  C18       3.1412903359     -1.5834726501     -2.0941408263
  C19       0.7612278937     -1.4867711375     -2.3895366683
  C20       1.7595442794     -0.4492050470     -0.4855736546
  C21       3.0091113795     -0.8573142142     -0.9207861868
  C22       2.0111531091     -1.8949252752     -2.8298034429
  H2       -0.1091069814     -1.7349751871     -2.9722862045
  H5        1.6838499759      0.1260797457      0.4187801335
  H7        3.8810755457     -0.6036854253     -0.3432863671
  H8        2.0984236266     -2.4527517657     -3.7455554517
  H9        4.1134804287     -1.8973501266     -2.4313683306
  H10      -1.4325022290     -0.4530199941     -1.6224471896
  H19      -0.3786465345     -3.1286331457     -0.0238742545
  H20      -1.8691356301     -2.9192463570     -0.9345116717
  H21      -1.9212588689     -3.2932948603      0.7852254724
  H22      -2.4352510523     -0.9256884813      0.4397311698
  H11       0.8082719992      1.3777452964      3.2319535410
  H12       0.3855259064     -0.2539988216      3.7554945791
  H13      -0.7666510989      1.0561691019      3.9618495265

  nuclear repulsion energy.......  1414.892408731 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  39   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
```

```
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    287    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3729
  grid # 3      214    214    212    217   7188
  grid # 4      211    211    209    218   9913

  end of program grid


  start of program rwr
```

```
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                        RMS     maximum
      e  d  i  u  i                        energy  density   DIIS
      r  t  s  t  d     total energy       change  change    error

etot  1  N  N  1  U  -783.03312721655                2.5E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03323038921  1.0E-04  1.2E-05  5.4E-04
etot  3  Y  Y  4  M  -783.03324325592  1.3E-05  3.7E-06  1.3E-04
etot  4  Y  N  4  M  -783.03324684579  3.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89240873069
   (E)  Total one-electron terms..... -3874.34964094500
   (I)  Total two-electron terms.....  1676.42398536852
   (L)  Electronic energy............. -2197.92565557647  (E+I)
   (N)  Total energy.................  -783.03324684579  (A+L)

 SCFE: SCF energy: HF    -783.03324684579 hartrees   iterations:
4


 HOMO energy:    -0.30210
 LUMO energy:     0.12929

  Orbital energies:
  -20.52664  -15.60058  -11.34619  -11.28620  -11.25659  -11.25009
  -11.24315  -11.24174  -11.24054  -11.23855  -11.23794  -11.23494
  -11.23121  -11.23055  -11.23000  -11.22953  -11.22851  -11.22780
  -11.20908   -1.39729   -1.26970   -1.16516   -1.14903   -1.10607
   -1.03012   -1.01871   -1.01796   -1.01270   -0.96258   -0.93279
   -0.85823   -0.83900   -0.83338   -0.82172   -0.79613   -0.74121
   -0.71100   -0.69502   -0.67286   -0.66435   -0.64467   -0.63756
   -0.62743   -0.61493   -0.61225   -0.60861   -0.59693   -0.58329
   -0.57639   -0.55346   -0.54884   -0.54068   -0.53096   -0.51904
   -0.51483   -0.50724   -0.50111   -0.49778   -0.48458   -0.46869
   -0.46290   -0.42163   -0.41155   -0.34266   -0.33292   -0.32298
   -0.30210    0.12929    0.13404    0.14443    0.15223    0.20384
    0.22972    0.24095    0.24891    0.26128    0.28802

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.562992E-05	4.768429E-05	-5.437436E-05
2	C1	-1.009371E-05	-3.789597E-05	6.328968E-05
3	C2	-1.554082E-05	-8.805784E-05	-3.004251E-05
4	C3	2.037550E-05	4.671296E-05	1.839170E-04
5	C4	-2.313895E-05	-1.037498E-05	-5.935525E-05
6	C5	-1.603701E-05	1.971255E-05	-8.542037E-07
7	C6	-5.149507E-05	3.838504E-05	-1.939451E-04
8	C7	4.762197E-05	1.142669E-04	3.875016E-05
9	H3	-4.685806E-05	1.042584E-04	-7.557016E-05
10	H4	-3.767657E-05	1.036683E-04	-3.812976E-06
11	H6	-1.364980E-05	3.053078E-05	4.632092E-05
12	C16	-3.612585E-05	2.953732E-04	8.776485E-05
13	C8	-1.510165E-04	-4.746715E-05	-3.961850E-05
14	N2	-1.997635E-05	-4.313210E-04	2.279572E-04
15	C9	3.370634E-06	4.633911E-05	-1.005992E-04
16	C10	-4.035891E-05	-2.011830E-04	7.246247E-05
17	O1	-3.805300E-05	4.085369E-04	-1.572180E-04
18	C23	-4.302758E-05	5.862178E-05	-1.710521E-05
19	C18	1.202718E-04	8.888050E-06	2.477044E-05
20	C19	9.469438E-05	-4.470146E-05	-6.208727E-05
21	C20	5.790482E-05	3.445663E-04	3.855048E-04
22	C21	1.011344E-04	1.298277E-04	2.624729E-04
23	C22	-1.575061E-04	5.401534E-05	-4.751537E-05
24	H2	-2.273267E-04	-5.883771E-05	-2.228345E-04
25	H5	-3.541218E-06	-2.619689E-04	-2.245003E-04
26	H7	-9.864508E-05	-2.780676E-05	-1.964737E-05
27	H8	-3.001095E-05	-4.691237E-05	-2.363508E-04
28	H9	-1.505870E-05	-6.483817E-06	-3.438453E-05
29	H10	-7.305589E-05	-4.458270E-06	-3.547612E-05
30	H19	-3.954433E-07	-1.816276E-07	-7.264602E-06
31	H20	-1.282365E-05	2.928371E-05	-3.191699E-05
32	H21	-5.220631E-05	5.009572E-06	3.820078E-05
33	H22	1.406335E-05	-3.918633E-06	-1.449447E-05
34	H11	9.569794E-05	1.382193E-04	1.669425E-05
35	H12	-2.495846E-05	2.094196E-04	-6.765888E-05
36	H13	-4.102502E-05	6.368358E-05	-6.809803E-06
total		-7.500968E-04	1.025434E-03	-2.953311E-04

```
 end of program der1b
```

```
  start of program geopt  40

  geometry optimization step 40
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0102680
   Cos(theta):   0.7316907

   Final level shift:  -6.7963341E-02

  energy change:           9.7616E-06 *  (  5.0000E-05 )
  gradient maximum:        8.7075E-04 .  (  4.5000E-04 )
  gradient rms:            1.7040E-04 *  (  3.0000E-04 )
  step size:   0.01027  trust radius:   0.01000
  displacement maximum:    5.9074E-03 .  (  1.8000E-03 )
  displacement rms:        9.2962E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0653E-05    geom step:   1.0268E-
02    full step:   1.0268E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     6.9144E-08     y:     4.6027E-04     z:    -3.8823E-05

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1805335361     1.8877177032    -2.2326900447
  C1       -1.0989413761     2.1206477583    -1.1845471450
  C2       -0.8858702548     2.6958444450     1.5031177762
  C3       -0.8786978569     1.0872031151    -0.2891875535
  C4       -1.2058110018     3.4349959755    -0.7610442619
  C5       -1.0997845571     3.7145544921     0.5890755078
  C6       -0.7678197764     1.3781930832     1.0722442862
  C7       -0.7862406321    -0.3521354376    -0.7565307288
  H3       -1.3722551693     4.2232857581    -1.4730731250
  H4       -1.1876864256     4.7269806895     0.9421773897
  H6       -0.8182471882     2.9341741294     2.5467965553
  C16       0.6135056875    -0.7637827925    -1.2107322145
  C8       -1.3970642415    -1.2500474689     0.3423772349
  N2       -0.5091423997     0.3386125970     1.9932197827
  C9       -0.7812691256    -0.9761705188     1.7046116841
  C10       0.0102592893     0.6562561850     3.3155832988
  O1       -0.5798386170    -1.8495955228     2.5002490637
  C23      -1.3856762090    -2.7418101192     0.0238340609
  C18       3.1406210180    -1.5866317700    -2.0930786786
  C19       0.7615069768    -1.4796007199    -2.3942477003
  C20       1.7592605136    -0.4570917337    -0.4804324652
```

```
  C21       3.0084210909     -0.8676329823     -0.9148885438
  C22       2.0110729907     -1.8891394500     -2.8341545981
  H2       -0.1086863136     -1.7225574593     -2.9807779579
  H5        1.6829835578      0.1093993201      0.4284382373
  H7        3.8795672188     -0.6220483550     -0.3331545825
  H8        2.0984951984     -2.4415119632     -3.7538068850
  H9        4.1122636035     -1.9025835229     -2.4299831999
  H10      -1.4327934370     -0.4534479685     -1.6219331402
  H19      -0.3757025633     -3.1283877781     -0.0213372987
  H20      -1.8648899950     -2.9201142325     -0.9342981171
  H21      -1.9194687138     -3.2936030001      0.7857735821
  H22      -2.4343392319     -0.9269350977      0.4401755313
  H11       0.8098205086      1.3820355823      3.2292636056
  H12       0.3904122578     -0.2493428454      3.7549612324
  H13      -0.7640683520      1.0589051653      3.9612496031

  nuclear repulsion energy.......  1414.896243065 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  40   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.334E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
```

```
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    208    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2864
  grid # 2      110    109    108    111   3729
  grid # 3      214    213    212    217   7189
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
```

```
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -783.03313505465           2.5E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03324085548  1.1E-04  1.2E-05  5.3E-04
etot   3  Y  Y  4  M  -783.03325810499  1.7E-05  3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03325674898 -1.4E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89624306538
   (E)  Total one-electron terms..... -3874.36616452129
   (I)  Total two-electron terms.....  1676.43666470692
   (L)  Electronic energy............. -2197.92949981436  (E+I)
   (N)  Total energy.................  -783.03325674898  (A+L)

 SCFE: SCF energy: HF    -783.03325674898 hartrees   iterations:
4


 HOMO energy:    -0.30203
 LUMO energy:     0.12928

  Orbital energies:
  -20.52692  -15.60009  -11.34578  -11.28574  -11.25660  -11.24981
  -11.24296  -11.24133  -11.24052  -11.23872  -11.23790  -11.23493
  -11.23148  -11.23061  -11.23017  -11.22982  -11.22870  -11.22760
  -11.20917   -1.39749   -1.26944   -1.16499   -1.14892   -1.10595
   -1.03000   -1.01861   -1.01779   -1.01270   -0.96255   -0.93266
   -0.85808   -0.83891   -0.83326   -0.82165   -0.79604   -0.74108
   -0.71093   -0.69497   -0.67281   -0.66427   -0.64458   -0.63752
   -0.62742   -0.61486   -0.61224   -0.60847   -0.59691   -0.58336
   -0.57624   -0.55338   -0.54873   -0.54064   -0.53098   -0.51904
   -0.51487   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
   -0.46284   -0.42149   -0.41149   -0.34253   -0.33295   -0.32283
   -0.30203    0.12928    0.13401    0.14451    0.15235    0.20400
    0.22968    0.24104    0.24884    0.26136    0.28825

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.393421E-05	1.495904E-05	3.624136E-05
2	C1	-2.993544E-05	1.042517E-04	-8.034008E-05
3	C2	-4.965037E-05	1.428792E-04	1.491431E-05
4	C3	-4.266436E-05	1.379320E-05	-2.074520E-04
5	C4	-1.895811E-05	6.824643E-05	4.017110E-05
6	C5	-2.147496E-05	4.228074E-05	-1.157916E-05
7	C6	4.152878E-05	3.676471E-05	1.582159E-04
8	C7	-1.053052E-04	-6.140876E-05	-5.305938E-05
9	H3	6.540027E-06	-4.182934E-05	5.896687E-05
10	H4	-2.895909E-06	-4.363394E-05	-1.196816E-05
11	H6	-3.354574E-05	3.107920E-05	-6.340310E-05
12	C16	-1.525843E-05	-2.419853E-04	-8.257592E-05
13	C8	1.261373E-04	1.101140E-04	1.924357E-05
14	N2	-5.103716E-05	4.892301E-04	-2.566227E-04
15	C9	-6.899764E-05	2.376007E-05	9.216899E-05
16	C10	1.042331E-05	2.113738E-04	-5.609563E-05
17	O1	-1.396245E-06	-3.449606E-04	1.541131E-04
18	C23	5.081856E-06	3.565355E-06	-8.253708E-06
19	C18	-1.446029E-04	4.989481E-05	-4.088218E-05
20	C19	-1.428463E-04	1.096594E-04	3.763468E-05
21	C20	-1.053055E-04	-2.718897E-04	-3.869824E-04
22	C21	-1.340657E-04	-6.189925E-05	-2.699845E-04
23	C22	1.132563E-04	3.399720E-06	2.487180E-05
24	H2	1.796122E-04	1.204883E-04	1.954416E-04
25	H5	-3.544587E-05	3.133785E-04	2.036240E-04
26	H7	6.075275E-05	8.086912E-05	1.107105E-05
27	H8	-1.038044E-05	9.902074E-05	2.037797E-04
28	H9	-2.482317E-05	6.428656E-05	1.744572E-05
29	H10	3.609239E-05	6.434611E-05	1.485271E-05
30	H19	-4.190547E-05	5.773811E-05	-9.413444E-06
31	H20	-3.163223E-05	3.067309E-05	1.123170E-05
32	H21	5.133330E-06	4.944988E-05	-5.413174E-05
33	H22	-6.274101E-05	6.191068E-05	-2.267721E-06
34	H11	-1.612747E-04	-6.414317E-05	-3.065062E-05
35	H12	-6.744612E-06	-1.456896E-04	5.326628E-05
36	H13	3.049344E-05	-1.928691E-05	-1.409492E-05
total		-7.417701E-04	1.100686E-03	-2.925029E-04

```
 end of program der1b


 start of program geopt  41

 geometry optimization step 41
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
```

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0101777
   Cos(theta):   0.7147691

   Final level shift:  -6.1593040E-02

  energy change:          -9.9032E-06 *  (  5.0000E-05 )
  gradient maximum:        8.5287E-04 .  (  4.5000E-04 )
  gradient rms:            1.6624E-04 *  (  3.0000E-04 )
  step size:   0.01018  trust radius:   0.01000
  displacement maximum:    5.8838E-03 .  (  1.8000E-03 )
  displacement rms:        9.2145E-04 *  (  1.2000E-03 )
  predicted energy change:    -9.8689E-06    geom step:   1.0178E-
02    full step:   1.0178E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -3.3058E-05     y:    -4.4784E-04     z:     5.3437E-05

  new geometry:
                                angstroms
  atom            x                 y                 z
  H1       -1.1779194569      1.8889190743     -2.2325450547
  C1       -1.0965597414      2.1213224656     -1.1843436975
  C2       -0.8842826501      2.6953080188      1.5039180805
  C3       -0.8779893517      1.0871839076     -0.2894104033
  C4       -1.2020389484      3.4355922621     -0.7600223844
  C5       -1.0964785719      3.7145197498      0.5902041193
  C6       -0.7673508929      1.3777139443      1.0724718383
  C7       -0.7864953099     -0.3524133302     -0.7566952418
  H3       -1.3669792349      4.2243277534     -1.4716328280
  H4       -1.1832694477      4.7267565406      0.9437783582
  H6       -0.8170796761      2.9332465482      2.5476093782
  C16       0.6132581946     -0.7650148349     -1.2102809781
  C8       -1.3981527064     -1.2497582811      0.3421041590
  N2       -0.5101315530      0.3378017092      1.9930531716
  C9       -0.7831069091     -0.9772737844      1.7048025276
  C10       0.0081587989      0.6533380860      3.3163582796
  O1       -0.5832439836     -1.8518648168      2.5000584053
  C23      -1.3883345260     -2.7414971700      0.0228419317
  C18       3.1413473127     -1.5836004707     -2.0940117441
  C19       0.7612969520     -1.4867798452     -2.3895098609
  C20       1.7595811743     -0.4492812678     -0.4854930170
  C21       3.0091495209     -0.8574472014     -0.9206550894
  C22       2.0112248403     -1.8949897207     -2.8297283011
  H2       -0.1090233117     -1.7349294510     -2.9723045158
  H5        1.6838780835      0.1260013018      0.4188598558
  H7        3.8811023209     -0.6038680701     -0.3431119147
  H8        2.0985088614     -2.4528051787     -3.7454869236
  H9        4.1135383329     -1.8975200913     -2.4311995176
  H10      -1.4324139127     -0.4529636013     -1.6225103797
```

```
  H19      -0.3787505034     -3.1286191478     -0.0238576683
  H20      -1.8691834224     -2.9191671428     -0.9345758210
  H21      -1.9214163230     -3.2931984611      0.7851654438
  H22      -2.4352878148     -0.9255769366      0.4396277133
  H11       0.8081898220      1.3781404188      3.2316877391
  H12       0.3865268617     -0.2539622335      3.7549876177
  H13      -0.7662801158      1.0555260192      3.9620788991

  nuclear repulsion energy.......  1414.891433463 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  41   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
273
```

```
  number of gridpoints:
     atom         O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1       111     74     89     88     88     89     89
71
  grid # 2       123     79     97     95     96     97     96
112
  grid # 3       257    149    183    183    182    184    183
212
  grid # 4       450    286    327    326    327    327    327
211

  number of gridpoints:
     atom         H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1        71     73     73     73     66     71     71
70
  grid # 2       111    118    118    118    106    108    110
108
  grid # 3       212    223    223    224    203    218    217
217
  grid # 4       207    223    224    224    196    212    216
215

  number of gridpoints:
     atom        H22    H11    H12    H13  total
  grid # 1        69     71     70     71   2863
  grid # 2       110    109    107    111   3729
  grid # 3       214    214    212    217   7188
  grid # 4       211    211    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS     maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03313014867           2.6E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03323324161  1.0E-04  1.2E-05  5.4E-04
etot   3  Y  Y  4  M  -783.03324631058  1.3E-05  3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03325020781  3.9E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
```

```
   (A)  Nuclear repulsion.....  1414.89143346315
   (E)  Total one-electron terms..... -3874.34758542581
   (I)  Total two-electron terms.....  1676.42290175486
   (L)  Electronic energy..... -2197.92468367096  (E+I)
   (N)  Total energy.............  -783.03325020781  (A+L)

 SCFE: SCF energy: HF    -783.03325020781 hartrees   iterations:
4


 HOMO energy:    -0.30210
 LUMO energy:     0.12929

  Orbital energies:
 -20.52663  -15.60058  -11.34618  -11.28619  -11.25659  -11.25010
 -11.24315  -11.24174  -11.24055  -11.23855  -11.23794  -11.23494
 -11.23121  -11.23056  -11.23000  -11.22954  -11.22851  -11.22781
 -11.20909   -1.39729   -1.26969   -1.16517   -1.14903   -1.10607
  -1.03012   -1.01871   -1.01796   -1.01270   -0.96257   -0.93279
  -0.85823   -0.83900   -0.83338   -0.82172   -0.79613   -0.74121
  -0.71100   -0.69502   -0.67286   -0.66436   -0.64467   -0.63756
  -0.62743   -0.61493   -0.61225   -0.60860   -0.59693   -0.58330
  -0.57639   -0.55347   -0.54884   -0.54068   -0.53096   -0.51904
  -0.51483   -0.50724   -0.50111   -0.49778   -0.48458   -0.46869
  -0.46290   -0.42162   -0.41155   -0.34266   -0.33292   -0.32298
  -0.30210    0.12929    0.13404    0.14443    0.15223    0.20387
   0.22972    0.24095    0.24892    0.26128    0.28804

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1     -2.589628E-05   4.771375E-05  -5.422353E-05
   2    C1     -9.844688E-06  -3.950029E-05   6.371030E-05
   3    C2     -1.324931E-05  -8.698254E-05  -2.966539E-05
   4    C3      2.042670E-05   4.755193E-05   1.841441E-04
   5    C4     -2.303785E-05  -9.507382E-06  -5.876744E-05
   6    C5     -1.637066E-05   1.989334E-05  -1.285701E-06
   7    C6     -5.338211E-05   3.509113E-05  -1.922205E-04
```

8	C7	3.810672E-05	1.082191E-04	4.296461E-05
9	H3	-4.695844E-05	1.045048E-04	-7.560364E-05
10	H4	-3.782441E-05	1.039499E-04	-3.542282E-06
11	H6	-1.315311E-05	3.027402E-05	4.667190E-05
12	C16	-2.584165E-05	2.906123E-04	7.882361E-05
13	C8	-1.552032E-04	-4.224373E-05	-3.919689E-05
14	N2	-1.892933E-05	-4.367407E-04	2.256161E-04
15	C9	5.147190E-06	4.613714E-05	-9.946703E-05
16	C10	-4.207567E-05	-1.980349E-04	6.908777E-05
17	O1	-3.746568E-05	4.123184E-04	-1.609230E-04
18	C23	-4.134224E-05	5.757862E-05	-1.548210E-05
19	C18	1.172188E-04	7.128067E-06	2.400170E-05
20	C19	9.709640E-05	-4.428564E-05	-6.046110E-05
21	C20	6.059363E-05	3.441373E-04	3.878179E-04
22	C21	1.004934E-04	1.318370E-04	2.636001E-04
23	C22	-1.577278E-04	5.573230E-05	-4.772553E-05
24	H2	-2.273518E-04	-5.907989E-05	-2.220542E-04
25	H5	-4.242219E-06	-2.619764E-04	-2.242762E-04
26	H7	-1.000372E-04	-2.785027E-05	-2.043161E-05
27	H8	-2.996361E-05	-4.694047E-05	-2.357157E-04
28	H9	-1.545821E-05	-6.476687E-06	-3.449483E-05
29	H10	-7.195446E-05	-4.394553E-06	-3.307921E-05
30	H19	-2.023906E-06	7.461956E-07	-7.124757E-06
31	H20	-1.308576E-05	2.876695E-05	-3.191347E-05
32	H21	-5.101382E-05	6.412169E-06	3.643457E-05
33	H22	1.587493E-05	-5.279562E-06	-1.408004E-05
34	H11	9.868093E-05	1.375884E-04	1.743532E-05
35	H12	-2.655831E-05	2.086310E-04	-6.739582E-05
36	H13	-4.381953E-05	6.539100E-05	-4.852382E-06
total		-7.501726E-04	1.020922E-03	-2.936745E-04

```
 end of program der1b


 start of program geopt  42

 geometry optimization step 42
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0102660
  Cos(theta):   0.7310363

  Final level shift:  -6.7884585E-02

 energy change:           6.5412E-06 *  (  5.0000E-05 )
 gradient maximum:        8.6717E-04 .  (  4.5000E-04 )
```

```
  gradient rms:            1.7027E-04 *  (  3.0000E-04 )
  step size:   0.01027  trust radius:   0.01000
  displacement maximum:    5.9225E-03 .  (  1.8000E-03 )
  displacement rms:        9.2944E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0635E-05    geom step:   1.0266E-
02    full step:   1.0266E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     7.6995E-06     y:     4.5947E-04     z:    -4.2645E-05

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1804954383     1.8877686372    -2.2327238316
  C1       -1.0989286409     2.1206826120    -1.1845750941
  C2       -0.8859965485     2.6958501052     1.5031121659
  C3       -0.8786443741     1.0872368669    -0.2892253927
  C4       -1.2058874151     3.4350187076    -0.7610504837
  C5       -1.0999446927     3.7145635099     0.5890799535
  C6       -0.7677984036     1.3782233034     1.0722080781
  C7       -0.7862046541    -0.3521151090    -0.7565488782
  H3       -1.3723605638     4.2233097812    -1.4730718021
  H4       -1.1879531856     4.7269758944     0.9421945900
  H6       -0.8184734365     2.9341483845     2.5468071062
  C16       0.6135572005    -0.7638109870    -1.2107091962
  C8       -1.3971113730    -1.2499858765     0.3423438881
  N2       -0.5090720355     0.3386321658     1.9931573014
  C9       -0.7813527639    -0.9761209362     1.7045983945
  C10       0.0105388121     0.6561991201     3.3154660142
  O1       -0.5800221869    -1.8495261394     2.5002844554
  C23      -1.3857548262    -2.7417514779     0.0238125673
  C18       3.1406680078    -1.5867303924    -2.0929843515
  C19       0.7615690602    -1.4796081880    -2.3942334053
  C20       1.7592955116    -0.4571697483    -0.4803589005
  C21       3.0084550290    -0.8677461983    -0.9147813496
  C22       2.0111354118    -1.8891806580    -2.8341095882
  H2       -0.1086155435    -1.7225132353    -2.9807972799
  H5        1.6830031559     0.1093135617     0.4285132672
  H7        3.8795917435    -0.6222097445    -0.3330114700
  H8        2.0985712390    -2.4415321630    -3.7537756779
  H9        4.1123113992    -1.9027085757    -2.4298633879
  H10      -1.4327205900    -0.4534136254    -1.6219759793
  H19      -0.3757937583    -3.1283591353    -0.0213216581
  H20      -1.8649477050    -2.9200541103    -0.9343312877
  H21      -1.9195871742    -3.2935191061     0.7857403682
  H22      -2.4343803473    -0.9268441244     0.4400975996
  H11       0.8097161484     1.3823854113     3.2290766885
  H12       0.3912560463    -0.2493193963     3.7545311353
  H13      -0.7637770712     1.0583244321     3.9614700437

  nuclear repulsion energy.......  1414.894938254 hartrees
```

```
  ------------------------------------------------
 /  end of geometry optimization iteration  42   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.334E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    208    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
```

```
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2864
  grid # 2      110    109    108    111   3729
  grid # 3      214    213    212    217   7189
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                          RMS    maximum
      t  p  i  c  r                          energy  density   DIIS
      e  d  i  u  i                          change  change    error
      r  t  s  t  d     total energy

etot  1  N  N  1  U  -783.03313494677                  2.6E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03324005415  1.1E-04  1.2E-05  5.3E-04
etot  3  Y  Y  4  M  -783.03325689753  1.7E-05  3.7E-06  1.3E-04
etot  4  Y  N  4  M  -783.03325554068 -1.4E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89493825417
   (E)  Total one-electron terms..... -3874.36360563108
   (I)  Total two-electron terms.....  1676.43541183623
   (L)  Electronic energy............. -2197.92819379485  (E+I)
   (N)  Total energy.................  -783.03325554068  (A+L)

 SCFE: SCF energy: HF    -783.03325554068 hartrees   iterations:
4
```

```
HOMO energy:    -0.30204
LUMO energy:     0.12928

 Orbital energies:
 -20.52691  -15.60008  -11.34578  -11.28574  -11.25660  -11.24981
 -11.24296  -11.24134  -11.24052  -11.23872  -11.23790  -11.23494
 -11.23148  -11.23061  -11.23017  -11.22982  -11.22870  -11.22760
 -11.20917   -1.39748   -1.26944   -1.16498   -1.14892   -1.10595
  -1.03000   -1.01861   -1.01779   -1.01270   -0.96255   -0.93266
  -0.85808   -0.83891   -0.83326   -0.82165   -0.79604   -0.74108
  -0.71093   -0.69497   -0.67281   -0.66427   -0.64458   -0.63752
  -0.62742   -0.61486   -0.61224   -0.60847   -0.59690   -0.58336
  -0.57624   -0.55338   -0.54873   -0.54064   -0.53098   -0.51904
  -0.51487   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
  -0.46284   -0.42148   -0.41148   -0.34253   -0.33295   -0.32283
  -0.30204    0.12928    0.13401    0.14451    0.15235    0.20400
   0.22968    0.24104    0.24885    0.26136    0.28825

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -1.376191E-05   1.459492E-05   3.648699E-05
  2    C1     -3.001596E-05   1.047948E-04  -8.044564E-05
  3    C2     -4.717440E-05   1.425771E-04   1.421861E-05
  4    C3     -4.449984E-05   1.296302E-05  -2.080757E-04
  5    C4     -1.874635E-05   6.728239E-05   4.030130E-05
  6    C5     -2.160847E-05   4.136742E-05  -1.125257E-05
  7    C6      3.760471E-05   3.700220E-05   1.591218E-04
  8    C7     -9.546494E-05  -5.642248E-05  -5.543236E-05
  9    H3      6.669959E-06  -4.206098E-05   5.911224E-05
 10    H4     -2.872196E-06  -4.376410E-05  -1.185424E-05
 11    H6     -3.302341E-05   3.038630E-05  -6.323548E-05
 12    C16    -2.388683E-05  -2.390854E-04  -7.582299E-05
 13    C8      1.271983E-04   1.065346E-04   2.054815E-05
 14    N2     -4.847264E-05   4.906421E-04  -2.506701E-04
 15    C9     -6.503284E-05   2.190193E-05   9.149241E-05
 16    C10     1.008071E-05   2.143463E-04  -5.875587E-05
```

```
  17    O1     -2.783975E-06  -3.465013E-04   1.522603E-04
  18    C23     2.034168E-06   3.553391E-06  -7.679801E-06

  19    C18    -1.455053E-04   5.149661E-05  -3.951323E-05
  20    C19    -1.426453E-04   1.098225E-04   3.670533E-05
  21    C20    -1.050125E-04  -2.725328E-04  -3.902726E-04
  22    C21    -1.332752E-04  -6.458291E-05  -2.727378E-04
  23    C22     1.157918E-04   3.239593E-06   2.546653E-05
  24    H2      1.795483E-04   1.198461E-04   1.952215E-04
  25    H5     -3.548134E-05   3.132271E-04   2.043913E-04
  26    H7      6.007185E-05   8.103000E-05   1.027594E-05
  27    H8     -1.059481E-05   9.964200E-05   2.055442E-04
  28    H9     -2.546998E-05   6.438353E-05   1.793658E-05
  29    H10     3.395041E-05   6.431989E-05   1.299952E-05
  30    H19    -3.999623E-05   5.723742E-05  -9.833149E-06
  31    H20    -3.090805E-05   3.111391E-05   1.138996E-05
  32    H21     4.767729E-06   4.871563E-05  -5.333217E-05
  33    H22    -6.293372E-05   6.271088E-05  -3.143072E-06
  34    H11    -1.592426E-04  -6.618768E-05  -3.124284E-05
  35    H12    -7.636060E-06  -1.448433E-04   5.234877E-05
  36    H13     2.685978E-05  -1.811813E-05  -1.491355E-05
 -----------   -------------  -------------  -------------
    total      -7.414670E-04   1.100633E-03  -2.923918E-04

  end of program der1b


  start of program geopt  43

  geometry optimization step 43
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0101815
   Cos(theta):   0.7152035

   Final level shift:  -6.1840964E-02

  energy change:          -5.3329E-06 *  (  5.0000E-05 )
  gradient maximum:        8.5252E-04 .  (  4.5000E-04 )
  gradient rms:            1.6624E-04 *  (  3.0000E-04 )
  step size:   0.01018  trust radius:   0.01000
  displacement maximum:    5.8894E-03 .  (  1.8000E-03 )
  displacement rms:        9.2179E-04 *  (  1.2000E-03 )
  predicted energy change:    -9.8905E-06    geom step:   1.0181E-
02    full step:   1.0181E-02
  molecular structure not yet converged...
```

center of mass moved by:
x: -3.2554E-05 y: -4.4937E-04 z: 5.4326E-05

new geometry:

atom	x	y	z
		angstroms	
H1	-1.1778765941	1.8889700959	-2.2325767378
C1	-1.0965471247	2.1213585286	-1.1843696235
C2	-0.8844069844	2.6953114343	1.5039148272
C3	-0.8779428238	1.0872182670	-0.2894450939
C4	-1.2021099558	3.4356146134	-0.7600259955
C5	-1.0966304316	3.7145270154	0.5902115206
C6	-0.7673405182	1.3777414403	1.0724401872
C7	-0.7864581320	-0.3523866174	-0.7567144398
H3	-1.3670732543	4.2243529026	-1.4716285007
H4	-1.1835189973	4.7267510897	0.9437982259
H6	-0.8172976384	2.9332180897	2.5476216989
C16	0.6132983488	-0.7650321227	-1.2102543616
C8	-1.3981872566	-1.2497050575	0.3420695992
N2	-0.5100715782	0.3378184895	1.9930013627
C9	-0.7831751996	-0.9772331714	1.7047879450
C10	0.0084223553	0.6532927049	3.3162456890
O1	-0.5834032877	-1.8518105522	2.5000826037
C23	-1.3884036227	-2.7414485478	0.0228174982
C18	3.1413894713	-1.5836947127	-2.0939206950
C19	0.7613496878	-1.4867818415	-2.3894944812
C20	1.7596121038	-0.4493514775	-0.4854255845
C21	3.0091801213	-0.8575561642	-0.9205556862
C22	2.0112800323	-1.8950279422	-2.8296824271
H2	-0.1089617317	-1.7348867726	-2.9723250778
H5	1.6839012632	0.1259211607	0.4189316837
H7	3.8811243680	-0.6040226281	-0.3429784087
H8	2.0985736182	-2.4528264061	-3.7454518205
H9	4.1135794065	-1.8976441091	-2.4310823397
H10	-1.4323470217	-0.4529238314	-1.6225539925
H19	-0.3788289516	-3.1286032092	-0.0238446188
H20	-1.8692247573	-2.9191104379	-0.9346158901
H21	-1.9215301198	-3.2931284864	0.7851269051
H22	-2.4353188310	-0.9254950910	0.4395491847
H11	0.8081090358	1.3784577400	3.2314922198
H12	0.3873046320	-0.2539282760	3.7545976418
H13	-0.7660034403	1.0550181873	3.9622666300

nuclear repulsion energy..... 1414.890396223 hartrees

```
/  end of geometry optimization iteration  43   /
```

end of program geopt

start of program onee

```
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
```

```
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3729
  grid # 3      214    214    212    217   7188
  grid # 4      211    211    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03312996490             2.6E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03323314850  1.0E-04    1.2E-05  5.4E-04
etot   3  Y  Y  4  M  -783.03324629841  1.3E-05    3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03324984523  3.5E-06    0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89039622303
   (E)  Total one-electron terms..... -3874.34551501109
   (I)  Total two-electron terms.....  1676.42186894284
   (L)  Electronic energy............. -2197.92364606826  (E+I)
   (N)  Total energy.................  -783.03324984523  (A+L)

 SCFE: SCF energy: HF    -783.03324984523 hartrees   iterations:
4


 HOMO energy:    -0.30211
 LUMO energy:     0.12929

  Orbital energies:
  -20.52663  -15.60057  -11.34618  -11.28619  -11.25659  -11.25010
  -11.24315  -11.24174  -11.24055  -11.23855  -11.23794  -11.23494
  -11.23121  -11.23056  -11.23000  -11.22954  -11.22851  -11.22781
```

```
-11.20909   -1.39728   -1.26969   -1.16517   -1.14903   -1.10607
 -1.03012   -1.01872   -1.01796   -1.01270   -0.96257   -0.93279
 -0.85822   -0.83900   -0.83338   -0.82172   -0.79613   -0.74121
 -0.71100   -0.69502   -0.67286   -0.66436   -0.64467   -0.63756
 -0.62743   -0.61493   -0.61225   -0.60860   -0.59693   -0.58330
 -0.57639   -0.55347   -0.54884   -0.54068   -0.53095   -0.51904
 -0.51483   -0.50724   -0.50111   -0.49778   -0.48458   -0.46869
 -0.46290   -0.42162   -0.41155   -0.34266   -0.33292   -0.32298
 -0.30211    0.12929    0.13404    0.14443    0.15223    0.20387
  0.22971    0.24095    0.24892    0.26128    0.28804

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.593313E-05	4.752226E-05	-5.400960E-05
2	C1	-9.722814E-06	-4.024917E-05	6.394110E-05
3	C2	-1.116491E-05	-8.678072E-05	-2.905445E-05
4	C3	1.869277E-05	4.726286E-05	1.850651E-04
5	C4	-2.284691E-05	-8.904572E-06	-5.836790E-05
6	C5	-1.677935E-05	2.006500E-05	-2.024272E-06
7	C6	-5.533760E-05	3.253833E-05	-1.904874E-04
8	C7	4.003288E-05	1.091781E-04	4.074114E-05
9	H3	-4.690792E-05	1.043981E-04	-7.542225E-05
10	H4	-3.780260E-05	1.038391E-04	-3.378706E-06
11	H6	-1.264257E-05	3.007227E-05	4.692390E-05
12	C16	-2.471120E-05	2.893177E-04	7.650634E-05
13	C8	-1.569064E-04	-4.337686E-05	-3.780526E-05
14	N2	-1.775391E-05	-4.369726E-04	2.246400E-04
15	C9	6.946956E-06	4.619689E-05	-1.000894E-04
16	C10	-4.319361E-05	-1.938107E-04	6.585427E-05
17	O1	-3.723769E-05	4.119163E-04	-1.616137E-04
18	C23	-4.115256E-05	5.774115E-05	-1.493980E-05
19	C18	1.160713E-04	7.068333E-06	2.316427E-05
20	C19	9.843168E-05	-4.366286E-05	-5.969005E-05
21	C20	6.010948E-05	3.436634E-04	3.862554E-04
22	C21	9.961180E-05	1.316857E-04	2.642514E-04
23	C22	-1.601284E-04	5.660090E-05	-4.647161E-05
24	H2	-2.259684E-04	-5.882404E-05	-2.210379E-04

```
  25    H5     -4.207347E-06  -2.619527E-04  -2.237184E-04
  26    H7     -1.002766E-04  -2.763245E-05  -2.064677E-05
  27    H8     -2.993417E-05  -4.659644E-05  -2.348585E-04
  28    H9     -1.489325E-05  -6.571709E-06  -3.455965E-05
  29    H10    -7.187510E-05  -4.418863E-06  -3.237203E-05
  30    H19    -2.797072E-06   1.166187E-06  -7.108444E-06
  31    H20    -1.297488E-05   2.879369E-05  -3.177992E-05
  32    H21    -5.051204E-05   6.964550E-06   3.600861E-05
  33    H22     1.691152E-05  -5.169720E-06  -1.418318E-05
  34    H11     1.007081E-04   1.366115E-04   1.773272E-05
  35    H12    -2.756829E-05   2.071524E-04  -6.709155E-05
  36    H13    -4.626406E-05   6.643862E-05  -3.946632E-06
 -----------   -------------  -------------  -------------
    total      -7.499763E-04   1.021270E-03  -2.935731E-04

  end of program der1b


  start of program geopt  44

  geometry optimization step 44
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0102626
   Cos(theta):   0.7304804

   Final level shift:  -6.7699058E-02

  energy change:           5.6955E-06 *  (  5.0000E-05 )
  gradient maximum:        8.6768E-04 .  (  4.5000E-04 )
  gradient rms:            1.7015E-04 *  (  3.0000E-04 )
  step size:   0.01026  trust radius:   0.01000
  displacement maximum:    5.9272E-03 .  (  1.8000E-03 )
  displacement rms:        9.2913E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0609E-05    geom step:   1.0263E-
02    full step:   1.0263E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.2441E-05     y:     4.5957E-04     z:    -4.5035E-05

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1804594668     1.8878103081    -2.2327523705
  C1       -1.0989185957     2.1207128205    -1.1845989513
  C2       -0.8861077787     2.6958553070     1.5031070810
```

```
 C3       -0.8786008920      1.0872667532     -0.2892562575
 C4       -1.2059546059      3.4350379220     -0.7610566113
 C5       -1.1000836777      3.7145711776      0.5890828258
 C6       -0.7677865045      1.3782487857      1.0721788765
 C7       -0.7861696283     -0.3520917413     -0.7565666694
 H3       -1.3724511832      4.2233295622     -1.4730722542
 H4       -1.1881812813      4.7269721358      0.9422077126
 H6       -0.8186682107      2.9341274366      2.5468155021
 C16       0.6135935501     -0.7638279342     -1.2106870893
 C8       -1.3971385423     -1.2499388497      0.3423159655
 N2       -0.5090177006      0.3386505145      1.9931090105
 C9       -0.7814102295     -0.9760810484      1.7045874734
 C10       0.0107665103      0.6561596353      3.3153692451
 O1       -0.5801554403     -1.8494712619      2.5003103902
 C23      -1.3858126082     -2.7417075592      0.0237951654
 C18       3.1407024337     -1.5868193226     -2.0929057556
 C19       0.7616158953     -1.4796015753     -2.3942250069
 C20       1.7593217134     -0.4572436325     -0.4802946062
 C21       3.0084799771     -0.8678564023     -0.9146879648
 C22       2.0111806401     -1.8892083872     -2.8340753403
 H2       -0.1085589393     -1.7224580739     -2.9808234584
 H5        1.6830222533      0.1092233447      0.4285863250
 H7        3.8796083834     -0.6223686824     -0.3328834810
 H8        2.0986249086     -2.4415375096     -3.7537565595
 H9        4.1123445194     -1.9028259836     -2.4297630674
 H10      -1.4326602898     -0.4533802709     -1.6220131910
 H19      -0.3758609365     -3.1283404360     -0.0213143832
 H20      -1.8649902244     -2.9200066563     -0.9343572507
 H21      -1.9196751467     -3.2934561641      0.7857156809
 H22      -2.4344035219     -0.9267714796      0.4400308613
 H11       0.8096346991      1.3826719653      3.2289179041
 H12       0.3919381852     -0.2492921436      3.7541843247
 H13      -0.7635390802      1.0578667656      3.9616435282

 nuclear repulsion energy.......  1414.894156743 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  44   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.334E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    208    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
```

```
  grid # 1       69     71     70     71   2864
  grid # 2      110    109    108    111   3729
  grid # 3      214    213    212    217   7189
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  1  U  -783.03313466064           2.6E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03324030772  1.1E-04  1.2E-05  5.3E-04
etot  3  Y  Y  4  M  -783.03325723312  1.7E-05  3.7E-06  1.3E-04
etot  4  Y  N  4  M  -783.03325577929 -1.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89415674291
   (E)  Total one-electron terms..... -3874.36205711246
   (I)  Total two-electron terms.....  1676.43464459026
   (L)  Electronic energy............. -2197.92741252220  (E+I)
   (N)  Total energy.................  -783.03325577929  (A+L)

 SCFE: SCF energy: HF    -783.03325577929 hartrees   iterations:
4


 HOMO energy:    -0.30204
 LUMO energy:     0.12928

  Orbital energies:
  -20.52691  -15.60008  -11.34577  -11.28574  -11.25660  -11.24981
  -11.24296  -11.24134  -11.24052  -11.23872  -11.23790  -11.23494
  -11.23148  -11.23061  -11.23017  -11.22982  -11.22870  -11.22760
  -11.20917   -1.39748   -1.26943   -1.16498   -1.14892   -1.10595
   -1.03000   -1.01861   -1.01779   -1.01270   -0.96254   -0.93266
   -0.85808   -0.83891   -0.83326   -0.82165   -0.79604   -0.74108
   -0.71093   -0.69497   -0.67281   -0.66427   -0.64458   -0.63752
   -0.62742   -0.61487   -0.61224   -0.60847   -0.59690   -0.58336
   -0.57624   -0.55339   -0.54873   -0.54063   -0.53098   -0.51904
   -0.51487   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
   -0.46284   -0.42148   -0.41148   -0.34253   -0.33295   -0.32283
   -0.30204    0.12928    0.13401    0.14451    0.15235    0.20401
```

```
   0.22968    0.24104    0.24885    0.26136    0.28826

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.374996E-05	1.444845E-05	3.658792E-05
2	C1	-2.989657E-05	1.047020E-04	-8.015220E-05
3	C2	-4.534906E-05	1.426150E-04	1.394123E-05
4	C3	-4.618557E-05	1.319810E-05	-2.083023E-04
5	C4	-1.856831E-05	6.695007E-05	4.023099E-05
6	C5	-2.167081E-05	4.074157E-05	-1.088725E-05
7	C6	3.501114E-05	3.696430E-05	1.602720E-04
8	C7	-9.382301E-05	-5.606039E-05	-5.539719E-05
9	H3	6.769898E-06	-4.213392E-05	5.925536E-05
10	H4	-2.861011E-06	-4.384241E-05	-1.171237E-05
11	H6	-3.260359E-05	2.999225E-05	-6.313540E-05
12	C16	-2.361513E-05	-2.387910E-04	-7.583739E-05
13	C8	1.258817E-04	1.063336E-04	2.106111E-05
14	N2	-4.640259E-05	4.910555E-04	-2.476111E-04
15	C9	-6.283859E-05	2.049213E-05	9.018169E-05
16	C10	9.130023E-06	2.169888E-04	-6.074603E-05
17	O1	-3.392537E-06	-3.472550E-04	1.510153E-04
18	C23	1.441184E-06	3.680549E-06	-7.437807E-06
19	C18	-1.466072E-04	5.226018E-05	-3.889968E-05
20	C19	-1.421842E-04	1.099595E-04	3.668641E-05
21	C20	-1.046247E-04	-2.728761E-04	-3.913034E-04
22	C21	-1.335176E-04	-6.588386E-05	-2.742847E-04
23	C22	1.173937E-04	3.245300E-06	2.587399E-05
24	H2	1.793192E-04	1.197155E-04	1.953869E-04
25	H5	-3.561795E-05	3.131992E-04	2.045730E-04
26	H7	5.947277E-05	8.105790E-05	9.700419E-06
27	H8	-1.079649E-05	1.002828E-04	2.070789E-04
28	H9	-2.581811E-05	6.453680E-05	1.817960E-05
29	H10	3.350872E-05	6.433806E-05	1.303009E-05
30	H19	-3.930182E-05	5.693530E-05	-9.932210E-06
31	H20	-3.067714E-05	3.130425E-05	1.142604E-05
32	H21	4.827666E-06	4.887153E-05	-5.321453E-05
33	H22	-6.257343E-05	6.294713E-05	-3.233179E-06

```
 34    H11    -1.573241E-04  -6.751858E-05  -3.152223E-05
 35    H12    -8.278252E-06  -1.445661E-04   5.193516E-05
 36    H13     2.423725E-05  -1.717051E-05  -1.509528E-05
-----------   -------------  -------------  -------------
   total      -7.412846E-04   1.100718E-03  -2.922882E-04

 end of program der1b


 start of program geopt  45

 geometry optimization step 45
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0101843
  Cos(theta):   0.7156641

  Final level shift:  -6.2018670E-02

 energy change:          -5.9341E-06 *  (  5.0000E-05 )
 gradient maximum:        8.5281E-04 .  (  4.5000E-04 )
 gradient rms:            1.6630E-04 *  (  3.0000E-04 )
 step size:   0.01018  trust radius:   0.01000
 displacement maximum:    5.8909E-03 .  (  1.8000E-03 )
 displacement rms:        9.2204E-04 *  (  1.2000E-03 )
 predicted energy change:    -9.9103E-06    geom step:   1.0184E-
02    full step:   1.0184E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -3.1802E-05     y:    -4.5080E-04     z:     5.4004E-05

 new geometry:
                                 angstroms
 atom            x                  y                  z
 H1       -1.1778415137      1.8890071417     -2.2326029098
 C1       -1.0965370151      2.1213857129     -1.1843914795
 C2       -0.8845088467      2.6953160757      1.5039104393
 C3       -0.8779056124      1.0872453269     -0.2894723877
 C4       -1.2021678482      3.4356315848     -0.7600322305
 C5       -1.0967542326      3.7145334952      0.5902138190
 C6       -0.7673332533      1.3777645933      1.0724148509
 C7       -0.7864272645     -0.3523651661     -0.7567297860
 H3       -1.3671494905      4.2243707776     -1.4716298171
 H4       -1.1837217723      4.7267476481      0.9438091546
 H6       -0.8174754280      2.9331990067      2.5476293690
 C16       0.6133299324     -0.7650461964     -1.2102337762
```

```
  C8       -1.3982114045     -1.2496636107      0.3420443914
  N2       -0.5100253345      0.3378348934      1.9929607513
  C9       -0.7832264604     -0.9771986801      1.7047781862
  C10       0.0086286418      0.6532600349      3.3161581105
  O1       -0.5835230169     -1.8517636361      2.5001046818
  C23      -1.3884522076     -2.7414100563      0.0228010800
  C18       3.1414207869     -1.5837741668     -2.0938497442
  C19       0.7613907921     -1.4867731976     -2.3894886861
  C20       1.7596354145     -0.4494193719     -0.4853666281
  C21       3.0092022373     -0.8576579252     -0.9204710044
  C22       2.0113211666     -1.8950501437     -2.8296527006
  H2       -0.1089129774     -1.7348339156     -2.9723515558
  H5        1.6839191098      0.1258361227      0.4190002872
  H7        3.8811389485     -0.6041703716     -0.3428613070
  H8        2.0986214419     -2.4528268628     -3.7454359378
  H9        4.1136093351     -1.8977495201     -2.4309910504
  H10      -1.4322934446     -0.4528936613     -1.6225871933
  H19      -0.3788845498     -3.1285872386     -0.0238368714
  H20      -1.8692563847     -2.9190675747     -0.9346418859
  H21      -1.9216078714     -3.2930741627      0.7851024488
  H22      -2.4353401065     -0.9254318628      0.4394890980
  H11       0.8080389672      1.3787165917      3.2313417702
  H12       0.3879219707     -0.2538980287      3.7542883390
  H13      -0.7657876788      1.0546135586      3.9624189591

  nuclear repulsion energy.......  1414.889640653 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  45   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
```

```
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3729
  grid # 3      214    214    212    217   7188
  grid # 4      211    211    209    218   9912

  end of program grid


  start of program rwr
```

```
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                        RMS     maximum
      e  d  i  u  i                        energy  density   DIIS
      r  t  s  t  d     total energy       change  change    error

etot  1  N  N  1  U  -783.03312974394                2.6E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03323319538  1.0E-04       1.2E-05  5.4E-04
etot  3  Y  Y  4  M  -783.03324635334  1.3E-05       3.7E-06  1.3E-04
etot  4  Y  N  4  M  -783.03324996818  3.6E-06       0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.88964065331
   (E)  Total one-electron terms..... -3874.34400733605
   (I)  Total two-electron terms.....  1676.42111671456
   (L)  Electronic energy............. -2197.92289062149  (E+I)
   (N)  Total energy.................  -783.03324996818  (A+L)

 SCFE: SCF energy: HF    -783.03324996818 hartrees   iterations:
4


 HOMO energy:    -0.30211
 LUMO energy:     0.12929

  Orbital energies:
  -20.52663  -15.60057  -11.34618  -11.28619  -11.25659  -11.25010
  -11.24315  -11.24175  -11.24055  -11.23855  -11.23794  -11.23494
  -11.23121  -11.23056  -11.23000  -11.22954  -11.22851  -11.22781
  -11.20909   -1.39728   -1.26969   -1.16517   -1.14903   -1.10607
   -1.03012   -1.01872   -1.01796   -1.01270   -0.96257   -0.93279
   -0.85822   -0.83900   -0.83338   -0.82172   -0.79613   -0.74121
   -0.71100   -0.69502   -0.67286   -0.66436   -0.64467   -0.63756
   -0.62743   -0.61493   -0.61225   -0.60860   -0.59692   -0.58330
   -0.57639   -0.55348   -0.54884   -0.54068   -0.53095   -0.51904
   -0.51483   -0.50723   -0.50111   -0.49778   -0.48458   -0.46869
   -0.46290   -0.42162   -0.41154   -0.34266   -0.33292   -0.32298
   -0.30211    0.12929    0.13404    0.14443    0.15222    0.20387
    0.22971    0.24095    0.24893    0.26128    0.28804

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.593197E-05	4.744537E-05	-5.379619E-05
2	C1	-9.615635E-06	-4.076573E-05	6.414691E-05
3	C2	-9.537623E-06	-8.658949E-05	-2.896425E-05
4	C3	1.735167E-05	4.737873E-05	1.853036E-04
5	C4	-2.269523E-05	-8.734416E-06	-5.812024E-05
6	C5	-1.702405E-05	1.997372E-05	-2.280607E-06
7	C6	-5.710676E-05	3.105719E-05	-1.893438E-04
8	C7	4.109482E-05	1.093106E-04	4.035450E-05
9	H3	-4.687446E-05	1.043752E-04	-7.527442E-05
10	H4	-3.781954E-05	1.038589E-04	-3.209037E-06
11	H6	-1.224717E-05	2.988169E-05	4.717140E-05
12	C16	-2.375881E-05	2.888080E-04	7.507849E-05
13	C8	-1.578700E-04	-4.351302E-05	-3.716241E-05
14	N2	-1.645269E-05	-4.373078E-04	2.250705E-04
15	C9	8.485128E-06	4.595655E-05	-1.006815E-04
16	C10	-4.387915E-05	-1.907708E-04	6.340120E-05
17	O1	-3.726744E-05	4.115989E-04	-1.624888E-04
18	C23	-4.131560E-05	5.762049E-05	-1.469610E-05
19	C18	1.149371E-04	7.178035E-06	2.296499E-05
20	C19	9.917560E-05	-4.333284E-05	-5.916228E-05
21	C20	6.003989E-05	3.431386E-04	3.852964E-04
22	C21	9.919148E-05	1.314184E-04	2.641726E-04
23	C22	-1.607724E-04	5.701543E-05	-4.591316E-05
24	H2	-2.252531E-04	-5.866784E-05	-2.204760E-04
25	H5	-4.248718E-06	-2.619024E-04	-2.234698E-04
26	H7	-1.004668E-04	-2.751029E-05	-2.086708E-05
27	H8	-2.990222E-05	-4.631079E-05	-2.340744E-04
28	H9	-1.475807E-05	-6.556654E-06	-3.450429E-05
29	H10	-7.210258E-05	-4.377440E-06	-3.206467E-05
30	H19	-2.984501E-06	1.315501E-06	-7.098188E-06
31	H20	-1.282843E-05	2.882525E-05	-3.166486E-05
32	H21	-5.025623E-05	7.263849E-06	3.580896E-05
33	H22	1.744947E-05	-5.113511E-06	-1.424059E-05
34	H11	1.022640E-04	1.356804E-04	1.778626E-05
35	H12	-2.841015E-05	2.064918E-04	-6.707158E-05
36	H13	-4.840131E-05	6.732414E-05	-3.405483E-06
total		-7.497915E-04	1.021464E-03	-2.934738E-04

```
 end of program der1b
```

```
  start of program geopt  46

  geometry optimization step 46
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0102598
   Cos(theta):   0.7300812

   Final level shift:  -6.7550790E-02

  energy change:           5.8111E-06 *  (  5.0000E-05 )
  gradient maximum:        8.6775E-04 .  (  4.5000E-04 )
  gradient rms:            1.7004E-04 *  (  3.0000E-04 )
  step size:   0.01026  trust radius:   0.01000
  displacement maximum:    5.9299E-03 .  (  1.8000E-03 )
  displacement rms:        9.2888E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0590E-05    geom step:   1.0260E-
02    full step:   1.0260E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.5401E-05     y:     4.5917E-04     z:    -4.6455E-05

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1804284623     1.8878422856    -2.2327760573
  C1       -1.0989099846     2.1207365745    -1.1846189531
  C2       -0.8862001817     2.6958607935     1.5031020895
  C3       -0.8785667722     1.0872909185    -0.2892807733
  C4       -1.2060085684     3.4350529892    -0.7610635728
  C5       -1.1001971534     3.7145778388     0.5890832466
  C6       -0.7677793812     1.3782703481     1.0721556811
  C7       -0.7861411061    -0.3520728342    -0.7565801186
  H3       -1.3725228593     4.2233447597    -1.4730753432
  H4       -1.1883669911     4.7269699206     0.9422155708
  H6       -0.8188291595     2.9341126054     2.5468212972
  C16       0.6136222858    -0.7638413217    -1.2106693278
  C8       -1.3971578520    -1.2499019925     0.3422949326
  N2       -0.5089765112     0.3386672124     1.9930722513
  C9       -0.7814540753    -0.9760481998     1.7045799059
  C10       0.0109477076     0.6561326949     3.3152922799
  O1       -0.5802575671    -1.8494260754     2.5003320198
  C23      -1.3858531301    -2.7416734271     0.0237828796
  C18       3.1407285589    -1.5868939710    -2.0928436185
  C19       0.7616528322    -1.4795879139    -2.3942235864
  C20       1.7593420390    -0.4573123788    -0.4802389848
```

```
  C21       3.0084985495     -0.8679568990     -0.9146091792
  C22       2.0112157901     -1.8892239940     -2.8340533675
  H2       -0.1085142040     -1.7223986126     -2.9808529554
  H5        1.6830375295      0.1091341259      0.4286536933
  H7        3.8796198042     -0.6225165111     -0.3327730156
  H8        2.0986662823     -2.4415290061     -3.7537502091
  H9        4.1123688874     -1.9029253991     -2.4296834396
  H10      -1.4326124822     -0.4533542197     -1.6220414679
  H19      -0.3759078611     -3.1283243092     -0.0213087768
  H20      -1.8650194685     -2.9199704870     -0.9343757649
  H21      -1.9197375534     -3.2934080764      0.7856985201
  H22      -2.4344203010     -0.9267159734      0.4399788708
  H11       0.8095670665      1.3829070826      3.2287885688
  H12       0.3924857097     -0.2492636744      3.7539081048
  H13      -0.7633497835      1.0575049204      3.9617823863

  nuclear repulsion energy.......  1414.893481698 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  46   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.334E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
```

```
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    208    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2864
  grid # 2      110    109    108    111   3729
  grid # 3      214    213    212    217   7189
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
```

```
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -783.03313451392           2.6E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03324018241  1.1E-04  1.2E-05  5.3E-04
etot   3  Y  Y  4  M  -783.03325716931  1.7E-05  3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03325565572 -1.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89348169850
   (E)  Total one-electron terms..... -3874.36071585881
   (I)  Total two-electron terms.....  1676.43397850459
   (L)  Electronic energy............. -2197.92673735422  (E+I)
   (N)  Total energy.................  -783.03325565572  (A+L)

 SCFE: SCF energy: HF    -783.03325565572 hartrees   iterations:
4


 HOMO energy:    -0.30204
 LUMO energy:     0.12928

  Orbital energies:
  -20.52691  -15.60008  -11.34577  -11.28574  -11.25661  -11.24981
  -11.24296  -11.24134  -11.24052  -11.23872  -11.23790  -11.23494
  -11.23148  -11.23061  -11.23017  -11.22982  -11.22870  -11.22760
  -11.20917   -1.39748   -1.26943   -1.16498   -1.14892   -1.10595
   -1.03000   -1.01861   -1.01779   -1.01270   -0.96254   -0.93266
   -0.85808   -0.83891   -0.83326   -0.82165   -0.79604   -0.74108
   -0.71093   -0.69497   -0.67280   -0.66427   -0.64458   -0.63751
   -0.62742   -0.61487   -0.61223   -0.60846   -0.59690   -0.58336
   -0.57624   -0.55339   -0.54873   -0.54063   -0.53097   -0.51904
   -0.51487   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
   -0.46284   -0.42148   -0.41148   -0.34253   -0.33295   -0.32283
   -0.30204    0.12928    0.13401    0.14451    0.15235    0.20401
    0.22968    0.24104    0.24885    0.26136    0.28826

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.374722E-05	1.435022E-05	3.667983E-05
2	C1	-2.981306E-05	1.045379E-04	-7.994755E-05
3	C2	-4.389091E-05	1.426727E-04	1.384270E-05
4	C3	-4.742565E-05	1.338239E-05	-2.084150E-04
5	C4	-1.842143E-05	6.685988E-05	4.034420E-05
6	C5	-2.178732E-05	4.038942E-05	-1.077428E-05
7	C6	3.305425E-05	3.657757E-05	1.612765E-04
8	C7	-9.282305E-05	-5.599587E-05	-5.531723E-05
9	H3	6.845914E-06	-4.222507E-05	5.938723E-05
10	H4	-2.838292E-06	-4.394467E-05	-1.161975E-05
11	H6	-3.225448E-05	2.969290E-05	-6.308130E-05
12	C16	-2.315069E-05	-2.386888E-04	-7.639412E-05
13	C8	1.248732E-04	1.062989E-04	2.149735E-05
14	N2	-4.480323E-05	4.912833E-04	-2.458287E-04
15	C9	-6.122018E-05	1.963679E-05	8.929448E-05
16	C10	8.309037E-06	2.192258E-04	-6.246822E-05
17	O1	-3.743349E-06	-3.477971E-04	1.501446E-04
18	C23	1.051980E-06	3.778395E-06	-7.221736E-06
19	C18	-1.475538E-04	5.261771E-05	-3.866425E-05
20	C19	-1.417895E-04	1.100661E-04	3.686879E-05
21	C20	-1.043207E-04	-2.732564E-04	-3.919495E-04
22	C21	-1.337913E-04	-6.654643E-05	-2.752043E-04
23	C22	1.182442E-04	3.365282E-06	2.622170E-05
24	H2	1.793282E-04	1.196664E-04	1.955954E-04
25	H5	-3.571373E-05	3.132209E-04	2.046819E-04
26	H7	5.912353E-05	8.112120E-05	9.341646E-06
27	H8	-1.089457E-05	1.007190E-04	2.081487E-04
28	H9	-2.597485E-05	6.464382E-05	1.833813E-05
29	H10	3.321299E-05	6.436604E-05	1.309302E-05
30	H19	-3.899135E-05	5.681417E-05	-9.957640E-06
31	H20	-3.050219E-05	3.141103E-05	1.146091E-05
32	H21	4.947446E-06	4.906085E-05	-5.322796E-05
33	H22	-6.223342E-05	6.306798E-05	-3.295364E-06
34	H11	-1.558242E-04	-6.856842E-05	-3.163976E-05
35	H12	-8.822737E-06	-1.445679E-04	5.169360E-05
36	H13	2.220932E-05	-1.640889E-05	-1.507576E-05
total		-7.411313E-04	1.100827E-03	-2.921717E-04

```
 end of program der1b


 start of program geopt  47

 geometry optimization step 47
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
```

```
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0101867
   Cos(theta):   0.7160862

   Final level shift:  -6.2173590E-02

  energy change:          -5.6875E-06 *  (  5.0000E-05 )
  gradient maximum:        8.5337E-04 .  (  4.5000E-04 )
  gradient rms:            1.6640E-04 *  (  3.0000E-04 )
  step size:   0.01019  trust radius:   0.01000
  displacement maximum:    5.8912E-03 .  (  1.8000E-03 )
  displacement rms:        9.2226E-04 *  (  1.2000E-03 )
  predicted energy change:    -9.9293E-06    geom step:   1.0187E-
02    full step:   1.0187E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -3.0518E-05     y:    -4.5178E-04     z:     5.3391E-05

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -1.1778121898     1.8890343030    -2.2326247997
  C1       -1.0965283967     2.1214061476    -1.1844101141
  C2       -0.8845919423     2.6953212681     1.5039052127
  C3       -0.8778757798     1.0872665291    -0.2894942106
  C4       -1.2022142923     3.4356443270    -0.7600399303
  C5       -1.0968545790     3.7145391977     0.5902127295
  C6       -0.7673281533     1.3777840854     1.0723943448
  C7       -0.7864022860    -0.3523488711    -0.7567410179
  H3       -1.3672103755     4.2243834251    -1.4716345487
  H4       -1.1838860044     4.7267456983     0.9438138962
  H6       -0.8176202754     2.9331864870     2.5476335121
  C16       0.6133549457    -0.7650582649    -1.2102176457
  C8       -1.3982285468    -1.2496312001     0.3420265823
  N2       -0.5099899580     0.3378502813     1.9929294263
  C9       -0.7832655242    -0.9771694888     1.7047723787
  C10       0.0087897447     0.6532373301     3.3160901280
  O1       -0.5836139907    -1.8517234908     2.5001247805
  C23      -1.3884866137    -2.7413802023     0.0227913350
  C18       3.1414442326    -1.5838399797    -2.0937951388
  C19       0.7614231093    -1.4867579530    -2.3894897550
  C20       1.7596533891    -0.4494837196    -0.4853153700
  C21       3.0092186897    -0.8577504744    -0.9203997140
  C22       2.0113526388    -1.8950604414    -2.8296356151
  H2       -0.1088741986    -1.7347758618    -2.9723816858
  H5        1.6839332016     0.1257508667     0.4190638931
  H7        3.8811491409    -0.6043076433    -0.3427601751
  H8        2.0986580660    -2.4528130678    -3.7454341696
  H9        4.1136312409    -1.8978370461    -2.4309207758
  H10      -1.4322513714    -0.4528713510    -1.6226117006
```

```
  H19      -0.3789239572     -3.1285729786     -0.0238300936
  H20      -1.8692796644     -2.9190359106     -0.9346577800
  H21      -1.9216621568     -3.2930323480      0.7850881007
  H22      -2.4353553639     -0.9253835787      0.4394436238
  H11       0.8079781859      1.3789279782      3.2312250985
  H12       0.3884119981     -0.2538700569      3.7540437915
  H13      -0.7656199502      1.0542924317      3.9625420498

  nuclear repulsion energy.......  1414.888983896 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  47   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
273
```

```
  number of gridpoints:
     atom         O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1       111     74     89     88     88     89     89
71
  grid # 2       123     79     97     95     96     97     96
112
  grid # 3       257    149    183    183    182    184    183
212
  grid # 4       450    286    327    326    327    327    327
211

  number of gridpoints:
     atom         H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1        71     73     73     73     66     71     71
70
  grid # 2       111    118    118    118    106    108    110
108
  grid # 3       212    223    223    224    203    218    217
217
  grid # 4       207    223    224    224    196    212    216
215

  number of gridpoints:
     atom        H22    H11    H12    H13  total
  grid # 1        69     71     70     71   2863
  grid # 2       110    109    107    111   3729
  grid # 3       214    214    212    217   7188
  grid # 4       211    211    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy       change  change    error

etot   1  N  N  1  U  -783.03312955143                2.6E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03323308852  1.0E-04       1.2E-05  5.4E-04
etot   3  Y  Y  4  M  -783.03324630294  1.3E-05       3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03324993704  3.6E-06       0.0E+00  0.0E+00


 Energy components, in hartrees:
```

```
   (A)  Nuclear repulsion.....  1414.88898389647
   (E)  Total one-electron terms..... -3874.34269638044
   (I)  Total two-electron terms.....  1676.42046254694
   (L)  Electronic energy..... -2197.92223383350  (E+I)
   (N)  Total energy.............  -783.03324993704  (A+L)

 SCFE: SCF energy: HF    -783.03324993704 hartrees   iterations:
4


 HOMO energy:    -0.30211
 LUMO energy:     0.12929

  Orbital energies:
 -20.52663  -15.60057  -11.34618  -11.28619  -11.25659  -11.25010
 -11.24315  -11.24175  -11.24055  -11.23855  -11.23794  -11.23494
 -11.23121  -11.23056  -11.23000  -11.22954  -11.22851  -11.22781
 -11.20909   -1.39728   -1.26969   -1.16516   -1.14903   -1.10607
  -1.03012   -1.01872   -1.01796   -1.01270   -0.96257   -0.93279
  -0.85822   -0.83900   -0.83338   -0.82172   -0.79613   -0.74121
  -0.71100   -0.69502   -0.67285   -0.66436   -0.64468   -0.63756
  -0.62743   -0.61493   -0.61225   -0.60860   -0.59692   -0.58330
  -0.57639   -0.55348   -0.54885   -0.54068   -0.53095   -0.51904
  -0.51483   -0.50723   -0.50111   -0.49778   -0.48458   -0.46869
  -0.46290   -0.42162   -0.41154   -0.34266   -0.33292   -0.32298
  -0.30211    0.12929    0.13404    0.14443    0.15222    0.20387
   0.22971    0.24095    0.24893    0.26128    0.28804

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1     -2.592724E-05   4.738559E-05  -5.364591E-05
   2    C1     -9.535754E-06  -4.117227E-05   6.429322E-05
   3    C2     -8.240798E-06  -8.645907E-05  -2.898460E-05
   4    C3      1.634745E-05   4.746618E-05   1.855231E-04
   5    C4     -2.257082E-05  -8.670732E-06  -5.793941E-05
   6    C5     -1.720519E-05   1.986566E-05  -2.422401E-06
   7    C6     -5.865622E-05   3.006689E-05  -1.884450E-04
```

```
 8    C7      4.191138E-05   1.094097E-04   4.019336E-05
 9    H3     -4.683814E-05   1.043592E-04  -7.516165E-05
10    H4     -3.782913E-05   1.038869E-04  -3.064837E-06
11    H6     -1.192879E-05   2.970364E-05   4.738680E-05
12    C16    -2.313426E-05   2.885947E-04   7.407104E-05
13    C8     -1.586582E-04  -4.360001E-05  -3.669174E-05
14    N2     -1.525597E-05  -4.374815E-04   2.258186E-04
15    C9      9.742382E-06   4.555393E-05  -1.012777E-04
16    C10    -4.430324E-05  -1.884428E-04   6.155559E-05
17    O1     -3.739803E-05   4.112932E-04  -1.632512E-04
18    C23    -4.153922E-05   5.760009E-05  -1.453023E-05
19    C18     1.140321E-04   7.277799E-06   2.290338E-05
20    C19     9.971514E-05  -4.316332E-05  -5.878721E-05
21    C20     6.018633E-05   3.426950E-04   3.846746E-04
22    C21     9.886890E-05   1.311615E-04   2.639256E-04
23    C22    -1.609215E-04   5.729772E-05  -4.554545E-05
24    H2     -2.248613E-04  -5.859888E-05  -2.201316E-04
25    H5     -4.328266E-06  -2.618403E-04  -2.232932E-04
26    H7     -1.006717E-04  -2.741190E-05  -2.108856E-05
27    H8     -2.989899E-05  -4.603152E-05  -2.333796E-04
28    H9     -1.472198E-05  -6.531845E-06  -3.443776E-05
29    H10    -7.231768E-05  -4.352805E-06  -3.188010E-05
30    H19    -3.013121E-06   1.365052E-06  -7.078438E-06
31    H20    -1.268627E-05   2.886360E-05  -3.158476E-05
32    H21    -5.007193E-05   7.493649E-06   3.567460E-05
33    H22     1.784926E-05  -5.056923E-06  -1.429418E-05
34    H11     1.035301E-04   1.349190E-04   1.776380E-05
35    H12    -2.910566E-05   2.061435E-04  -6.714745E-05
36    H13    -5.016299E-05   6.802679E-05  -3.091807E-06
-----------   -------------  -------------  -------------
  total       -7.495994E-04   1.021616E-03  -2.933711E-04

 end of program der1b


 start of program geopt  48

 geometry optimization step 48
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0102575
  Cos(theta):   0.7297533

  Final level shift:  -6.7425209E-02

 energy change:           5.7187E-06 *  (  5.0000E-05 )
 gradient maximum:        8.6762E-04 .  (  4.5000E-04 )
```

```
  gradient rms:            1.6996E-04 *  (  3.0000E-04 )
  step size:   0.01026  trust radius:   0.01000
  displacement maximum:    5.9312E-03 .  (  1.8000E-03 )
  displacement rms:        9.2867E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.0573E-05    geom step:   1.0258E-
02    full step:   1.0258E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.7185E-05     y:     4.5860E-04     z:    -4.7243E-05

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -1.1804020219     1.8878654324    -2.2327960356
  C1       -1.0989024297     2.1207542006    -1.1846361268
  C2       -0.8862758939     2.6958662600     1.5030965429
  C3       -0.8785397887     1.0873097429    -0.2893003140
  C4       -1.2060514031     3.4350639823    -0.7610717202
  C5       -1.1002889302     3.7145833482     0.5890809071
  C6       -0.7677749682     1.3782883375     1.0721370327
  C7       -0.7861183547    -0.3520585285    -0.7565898484
  H3       -1.3725791126     4.2233552018    -1.4730812957
  H4       -1.1885169840     4.7269686379     0.9422181395
  H6       -0.8189607512     2.9341026943     2.5468242049
  C16       0.6136448512    -0.7638526144    -1.2106550505
  C8       -1.3971720621    -1.2498731566     0.3422799256
  N2       -0.5089451168     0.3386823184     1.9930443293
  C9       -0.7814879789    -0.9760209907     1.7045754320
  C10       0.0110918852     0.6561146997     3.3152313388
  O1       -0.5803365035    -1.8493884743     2.5003510636
  C23      -1.3858820186    -2.7416469258     0.0237755021
  C18       3.1407485133    -1.5869549409    -2.0927949910
  C19       0.7616822142    -1.4795692921    -2.3942274276
  C20       1.7593574054    -0.4573761764    -0.4801902619
  C21       3.0085121210    -0.8680468254    -0.9145423921
  C22       2.0112436165    -1.8892291084    -2.8340412322
  H2       -0.1084782958    -1.7223369362    -2.9808848268
  H5        1.6830488478     0.1090473790     0.4287159209
  H7        3.8796271483    -0.6226514103    -0.3326772403
  H8        2.0986992437    -2.4415086204    -3.7537541595
  H9        4.1123871646    -1.9030068003    -2.4296209546
  H10      -1.4325749945    -0.4533349899    -1.6220625104
  H19      -0.3759410599    -3.1283106479    -0.0213026287
  H20      -1.8650395553    -2.9199431934    -0.9343879061
  H21      -1.9197826448    -3.2933711651     0.7856877655
  H22      -2.4344329674    -0.9266735849     0.4399391278
  H11       0.8095113671     1.3830992876     3.2286842424
  H12       0.3929242550    -0.2492362420     3.7536883933
  H13      -0.7631991565     1.0572189713     3.9618937245

  nuclear repulsion energy.......  1414.892904068 hartrees
```

```
  ------------------------------------------------
 /  end of geometry optimization iteration  48   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.334E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    208    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
```

```
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2864
  grid # 2      110    109    108    111   3729
  grid # 3      214    213    212    217   7189
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                              energy  density   DIIS
       e  d  i  u  i                              change  change    error
       r  t  s  t  d     total energy

etot   1  N  N  1  U  -783.03313441972                    2.6E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03324005258  1.1E-04  1.2E-05  5.3E-04
etot   3  Y  Y  4  M  -783.03325706295  1.7E-05  3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03325550569 -1.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89290406796
   (E)  Total one-electron terms..... -3874.35956759017
   (I)  Total two-electron terms.....  1676.43340801652
   (L)  Electronic energy............. -2197.92615957365  (E+I)
   (N)  Total energy.................  -783.03325550569  (A+L)

 SCFE: SCF energy: HF    -783.03325550569 hartrees   iterations:
4
```

```
HOMO energy:    -0.30204
LUMO energy:     0.12928

 Orbital energies:
 -20.52691  -15.60008  -11.34577  -11.28574  -11.25661  -11.24981
 -11.24296  -11.24134  -11.24052  -11.23872  -11.23790  -11.23494
 -11.23148  -11.23062  -11.23017  -11.22982  -11.22870  -11.22760
 -11.20917   -1.39748   -1.26943   -1.16498   -1.14892   -1.10594
  -1.03000   -1.01861   -1.01779   -1.01270   -0.96254   -0.93266
  -0.85808   -0.83891   -0.83326   -0.82165   -0.79604   -0.74108
  -0.71093   -0.69497   -0.67280   -0.66427   -0.64458   -0.63751
  -0.62742   -0.61487   -0.61223   -0.60846   -0.59690   -0.58336
  -0.57624   -0.55339   -0.54873   -0.54063   -0.53097   -0.51905
  -0.51487   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
  -0.46284   -0.42148   -0.41148   -0.34253   -0.33295   -0.32284
  -0.30204    0.12928    0.13401    0.14451    0.15235    0.20401
   0.22968    0.24104    0.24886    0.26136    0.28826

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x             y             z
----  -----   -------------  -------------  -------------
  1    H1     -1.374094E-05   1.428308E-05   3.678924E-05
  2    C1     -2.976425E-05   1.043472E-04  -7.981611E-05
  3    C2     -4.274820E-05   1.427553E-04   1.377841E-05
  4    C3     -4.834898E-05   1.350085E-05  -2.084144E-04
  5    C4     -1.830678E-05   6.684689E-05   4.048000E-05
  6    C5     -2.189754E-05   4.014377E-05  -1.074118E-05
  7    C6      3.155117E-05   3.607113E-05   1.620982E-04
  8    C7     -9.209072E-05  -5.594169E-05  -5.531487E-05
  9    H3      6.903323E-06  -4.229398E-05   5.950008E-05
 10    H4     -2.819135E-06  -4.401043E-05  -1.153511E-05
 11    H6     -3.197335E-05   2.949138E-05  -6.299610E-05
 12    C16    -2.275321E-05  -2.386365E-04  -7.697404E-05
 13    C8      1.241506E-04   1.062405E-04   2.188466E-05
 14    N2     -4.355120E-05   4.913537E-04  -2.448509E-04
 15    C9     -6.002501E-05   1.910663E-05   8.871172E-05
 16    C10     7.611018E-06   2.210285E-04  -6.395030E-05
```

```
  17    O1     -3.966842E-06  -3.481801E-04   1.494600E-04
  18    C23     7.992412E-07   3.805490E-06  -7.062397E-06
  19    C18    -1.483003E-04   5.281095E-05  -3.856095E-05
  20    C19    -1.414597E-04   1.101433E-04   3.709553E-05
  21    C20    -1.040785E-04  -2.736102E-04  -3.924379E-04
  22    C21    -1.340463E-04  -6.693595E-05  -2.757977E-04
  23    C22     1.187189E-04   3.502178E-06   2.650154E-05
  24    H2      1.794333E-04   1.196351E-04   1.958112E-04
  25    H5     -3.578795E-05   3.132449E-04   2.047664E-04
  26    H7      5.889452E-05   8.120446E-05   9.085483E-06
  27    H8     -1.095325E-05   1.010331E-04   2.089246E-04
  28    H9     -2.606901E-05   6.472350E-05   1.844767E-05
  29    H10     3.300206E-05   6.439903E-05   1.318336E-05
  30    H19    -3.890053E-05   5.678424E-05  -9.941576E-06
  31    H20    -3.035856E-05   3.147628E-05   1.151984E-05
  32    H21     5.083246E-06   4.924626E-05  -5.329808E-05
  33    H22    -6.191764E-05   6.315510E-05  -3.347798E-06
  34    H11    -1.546144E-04  -6.938276E-05  -3.170349E-05
  35    H12    -9.278418E-06  -1.446579E-04   5.154111E-05
  36    H13     2.059595E-05  -1.576104E-05  -1.495362E-05
 -----------   -------------  -------------  -------------
    total      -7.410075E-04   1.100922E-03  -2.921176E-04

  end of program der1b


  start of program geopt  49

  geometry optimization step 49
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0101888
   Cos(theta):   0.7164571

   Final level shift:  -6.2308517E-02

  energy change:          -5.5687E-06 *  (  5.0000E-05 )
  gradient maximum:        8.5395E-04 .  (  4.5000E-04 )
  gradient rms:            1.6649E-04 *  (  3.0000E-04 )
  step size:   0.01019  trust radius:   0.01000
  displacement maximum:    5.8911E-03 .  (  1.8000E-03 )
  displacement rms:        9.2245E-04 *  (  1.2000E-03 )
  predicted energy change:    -9.9462E-06    geom step:   1.0189E-
02    full step:   1.0189E-02
  molecular structure not yet converged...

  center of mass moved by:
```

```
   x:    -2.9157E-05     y:    -4.5250E-04     z:     5.2721E-05

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1777873031     1.8890534233    -2.2326433005
 C1       -1.0965208299     2.1214209574    -1.1844262261
 C2       -0.8846598180     2.6953266249     1.5038992819
 C3       -0.8778517744     1.0872828329    -0.2895116848
 C4       -1.2022513242     3.4356534154    -0.7600487784
 C5       -1.0969358926     3.7145440410     0.5902089926
 C6       -0.7673246952     1.3778004046     1.0723776061
 C7       -0.7863822285    -0.3523369228    -0.7567489120
 H3       -1.3672586339     4.2243916973    -1.4716419361
 H4       -1.1840190457     4.7267447288     0.9438138295
 H6       -0.8177385502     2.9331788258     2.5476348920
 C16       0.6133746411    -0.7650688679    -1.2102046732
 C8       -1.3982408656    -1.2496059753     0.3420144785
 N2       -0.5099629628     0.3378644275     1.9929052660
 C9       -0.7832956038    -0.9771448788     1.7047695127
 C10       0.0089166219     0.6532223060     3.3160367395
 O1       -0.5836836281    -1.8516892722     2.5001430785
 C23      -1.3885110351    -2.7413571986     0.0227866891
 C18       3.1414619079    -1.5838936719    -2.0937530744
 C19       0.7614487390    -1.4867380938    -2.3894956401
 C20       1.7596670084    -0.4495443691    -0.4852700174
 C21       3.0092307177    -0.8578339047    -0.9203390215
 C22       2.0113771878    -1.8950611329    -2.8296278900
 H2       -0.1088430027    -1.7347151171    -2.9724141015
 H5        1.6839437511     0.1256668845     0.4191233128
 H7        3.8811558350    -0.6044337885    -0.3426720292
 H8        2.0986868442    -2.4527880580    -3.7454426755
 H9        4.1136474152    -1.8979084312    -2.4308667050
 H10      -1.4322184566    -0.4528553947    -1.6226294530
 H19      -0.3789518713    -3.1285608775    -0.0238226035
 H20      -1.8692960468    -2.9190126722    -0.9346667199
 H21      -1.9217007830    -3.2930001938     0.7850806648
 H22      -2.4353665120    -0.9253467710     0.4394093949
 H11       0.8079272435     1.3791004544     3.2311328952
 H12       0.3888019816    -0.2538440821     3.7538500570
 H13      -0.7654879489     1.0540388559     3.9626410377

 nuclear repulsion energy.......  1414.888433943 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  49   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.335E-04
```

```
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    293
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
```

```
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3729
  grid # 3      214    214    212    217   7188
  grid # 4      211    211    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03312941788           2.6E-05  1.3E-03
etot   2  Y  Y  4  M  -783.03323292850  1.0E-04  1.2E-05  5.4E-04
etot   3  Y  Y  4  M  -783.03324616135  1.3E-05  3.7E-06  1.3E-04
etot   4  Y  N  4  M  -783.03324965978  3.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.88843394285
   (E)  Total one-electron terms..... -3874.34159995875
   (I)  Total two-electron terms.....  1676.41991635612
   (L)  Electronic energy............. -2197.92168360263  (E+I)
   (N)  Total energy.................  -783.03324965978  (A+L)

 SCFE: SCF energy: HF    -783.03324965978 hartrees   iterations:
4


 HOMO energy:    -0.30211
 LUMO energy:     0.12929

  Orbital energies:
  -20.52663  -15.60057  -11.34617  -11.28619  -11.25659  -11.25010
  -11.24315  -11.24175  -11.24056  -11.23855  -11.23794  -11.23494
  -11.23121  -11.23056  -11.23000  -11.22954  -11.22851  -11.22781
```

```
-11.20909   -1.39728   -1.26969   -1.16516   -1.14903   -1.10607
 -1.03012   -1.01872   -1.01796   -1.01270   -0.96257   -0.93279
 -0.85822   -0.83900   -0.83338   -0.82172   -0.79613   -0.74121
 -0.71100   -0.69502   -0.67285   -0.66436   -0.64468   -0.63756
 -0.62743   -0.61493   -0.61225   -0.60860   -0.59692   -0.58330
 -0.57639   -0.55348   -0.54885   -0.54068   -0.53095   -0.51904
 -0.51483   -0.50723   -0.50111   -0.49778   -0.48458   -0.46869
 -0.46290   -0.42161   -0.41154   -0.34266   -0.33293   -0.32298
 -0.30211    0.12929    0.13404    0.14443    0.15222    0.20387
  0.22971    0.24095    0.24893    0.26128    0.28804

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.592608E-05	4.732803E-05	-5.355182E-05
2	C1	-9.475848E-06	-4.145662E-05	6.443900E-05
3	C2	-7.193273E-06	-8.636665E-05	-2.900163E-05
4	C3	1.554508E-05	4.753995E-05	1.856340E-04
5	C4	-2.247090E-05	-8.627248E-06	-5.778068E-05
6	C5	-1.733481E-05	1.973921E-05	-2.518020E-06
7	C6	-5.998248E-05	2.940101E-05	-1.877519E-04
8	C7	4.253817E-05	1.094845E-04	4.014761E-05
9	H3	-4.680272E-05	1.043327E-04	-7.507083E-05
10	H4	-3.783413E-05	1.038886E-04	-2.961813E-06
11	H6	-1.166691E-05	2.953540E-05	4.753827E-05
12	C16	-2.268233E-05	2.885075E-04	7.330086E-05
13	C8	-1.593011E-04	-4.362636E-05	-3.633449E-05
14	N2	-1.420186E-05	-4.375676E-04	2.266601E-04
15	C9	1.074064E-05	4.515209E-05	-1.018360E-04
16	C10	-4.466173E-05	-1.865961E-04	6.009028E-05
17	O1	-3.753467E-05	4.110224E-04	-1.638338E-04
18	C23	-4.175842E-05	5.757407E-05	-1.443524E-05
19	C18	1.133071E-04	7.361266E-06	2.289409E-05
20	C19	1.001185E-04	-4.308707E-05	-5.851173E-05
21	C20	6.038344E-05	3.423298E-04	3.842122E-04
22	C21	9.862001E-05	1.309287E-04	2.636499E-04
23	C22	-1.608860E-04	5.750478E-05	-4.527604E-05
24	H2	-2.246100E-04	-5.857053E-05	-2.198800E-04

```
 25    H5     -4.410337E-06  -2.617838E-04  -2.231456E-04
 26    H7     -1.008692E-04  -2.732879E-05  -2.129666E-05
 27    H8     -2.990791E-05  -4.577584E-05  -2.327820E-04
 28    H9     -1.472450E-05  -6.500511E-06  -3.437616E-05
 29    H10    -7.248776E-05  -4.328403E-06  -3.175907E-05
 30    H19    -3.005584E-06   1.379870E-06  -7.054430E-06
 31    H20    -1.255258E-05   2.889833E-05  -3.151539E-05
 32    H21    -4.991861E-05   7.688394E-06   3.556840E-05
 33    H22     1.816219E-05  -5.003267E-06  -1.434331E-05
 34    H11     1.045549E-04   1.342958E-04   1.771052E-05
 35    H12    -2.966117E-05   2.059216E-04  -6.724378E-05
 36    H13    -5.161293E-05   6.858142E-05  -2.891794E-06
-----------   -------------  -------------  -------------
   total      -7.495037E-04   1.021777E-03  -2.933070E-04

 end of program der1b


 start of program geopt  50

 geometry optimization step 50
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0102556
  Cos(theta):   0.7294628

  Final level shift:  -6.7314654E-02

 energy change:           5.8459E-06 *  (  5.0000E-05 )
 gradient maximum:        8.6738E-04 .  (  4.5000E-04 )
 gradient rms:            1.6989E-04 *  (  3.0000E-04 )
 step size:   0.01026  trust radius:   0.01000
 displacement maximum:    5.9319E-03 .  (  1.8000E-03 )
 displacement rms:        9.2850E-04 *  (  1.2000E-03 )
 predicted energy change:    -1.0559E-05    geom step:   1.0256E-
02    full step:   1.0256E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:     1.8354E-05     y:     4.5806E-04     z:    -4.7718E-05

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1803789856     1.8878813188    -2.2328130744
 C1       -1.0988953563     2.1207667248    -1.1846510925
 C2       -0.8863376449     2.6958716269     1.5030904307
```

```
 C3       -0.8785181702      1.0873240508     -0.2893159703
 C4       -1.2060847899      3.4350715788     -0.7610808821
 C5       -1.1003626469      3.7145878349      0.5890762365
 C6       -0.7677723124      1.3783033444      1.0721218450
 C7       -0.7861001903     -0.3520482930     -0.7565964104
 H3       -1.3726224823      4.2233616793     -1.4730896066
 H4       -1.1886375146      4.7269680088      0.9422163490
 H6       -0.8190681086      2.9340967799      2.5468246515
 C16       0.6136625402     -0.7638626080     -1.2106434266
 C8       -1.3971823449     -1.2498508510      0.3422700235
 N2       -0.5089216278      0.3386960755      1.9930232048
 C9       -0.7815144796     -0.9759982062      1.7045737438
 C10       0.0112054067      0.6561035644      3.3151834148
 O1       -0.5803977148     -1.8493565871      2.5003687402
 C23      -1.3859019739     -2.7416267020      0.0237726206
 C18       3.1407636183     -1.5870041079     -2.0927579555
 C19       0.7617055082     -1.4795471289     -2.3942352335
 C20       1.7593689783     -0.4574358918     -0.4801472402
 C21       3.0085219220     -0.8681273289     -0.9144859062
 C22       2.0112655331     -1.8892256303     -2.8340372692
 H2       -0.1084495029     -1.7222742708     -2.9809180966
 H5        1.6830571597      0.1089628864      0.4287736924
 H7        3.8796316209     -0.6227743528     -0.3325943642
 H8        2.0987253483     -2.4414784436     -3.7537667891
 H9        4.1124006906     -1.9030722729     -2.4295734589
 H10      -1.4325456513     -0.4533215443     -1.6220775828
 H19      -0.3759638203     -3.1282991979     -0.0212948649
 H20      -1.8650523143     -2.9199234243     -0.9343944902
 H21      -1.9198145436     -3.2933430830      0.7856826164
 H22      -2.4344424009     -0.9266416255      0.4399092185
 H11       0.8094645910      1.3832565660      3.2286008575
 H12       0.3932737828     -0.2492102220      3.7535144108
 H13      -0.7630806805      1.0569937541      3.9619830161

 nuclear repulsion energy.......  1414.892408523 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  50   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.334E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
78
  grid # 3      223    223    207    194    174    211    176
146
  grid # 4      224    223    208    342    311    387    293
276

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
```

```
  grid # 1       69     71     70     71   2864
  grid # 2      110    109    108    111   3729
  grid # 3      214    213    212    217   7189
  grid # 4      211    211    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  1  U  -783.03313436264           2.6E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03323971206  1.1E-04  1.2E-05  5.3E-04
etot  3  Y  Y  4  M  -783.03325671957  1.7E-05  3.7E-06  1.3E-04
etot  4  Y  N  4  M  -783.03325513693 -1.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89240852303
   (E)  Total one-electron terms..... -3874.35858082590
   (I)  Total two-electron terms.....  1676.43291716594
   (L)  Electronic energy............. -2197.92566365996  (E+I)
   (N)  Total energy.................  -783.03325513693  (A+L)

 SCFE: SCF energy: HF    -783.03325513693 hartrees   iterations:
4


 HOMO energy:    -0.30204
 LUMO energy:     0.12928

  Orbital energies:
  -20.52691  -15.60008  -11.34577  -11.28574  -11.25661  -11.24981
  -11.24296  -11.24134  -11.24052  -11.23872  -11.23791  -11.23494
  -11.23148  -11.23062  -11.23018  -11.22982  -11.22870  -11.22760
  -11.20917   -1.39748   -1.26943   -1.16498   -1.14892   -1.10594
   -1.03000   -1.01861   -1.01779   -1.01270   -0.96254   -0.93266
   -0.85808   -0.83891   -0.83326   -0.82165   -0.79604   -0.74108
   -0.71093   -0.69497   -0.67280   -0.66427   -0.64458   -0.63751
   -0.62742   -0.61487   -0.61223   -0.60846   -0.59690   -0.58336
   -0.57624   -0.55339   -0.54873   -0.54063   -0.53097   -0.51905
   -0.51487   -0.50717   -0.50097   -0.49774   -0.48457   -0.46861
   -0.46284   -0.42148   -0.41148   -0.34253   -0.33296   -0.32284
   -0.30204    0.12928    0.13401    0.14451    0.15235    0.20401
```

```
   0.22968    0.24104    0.24886    0.26136    0.28826

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.373949E-05	1.423061E-05	3.687033E-05
2	C1	-2.973161E-05	1.041770E-04	-7.971008E-05
3	C2	-4.181288E-05	1.428732E-04	1.371293E-05
4	C3	-4.907179E-05	1.357117E-05	-2.083892E-04
5	C4	-1.821463E-05	6.685944E-05	4.060026E-05
6	C5	-2.199767E-05	3.997837E-05	-1.075045E-05
7	C6	3.034795E-05	3.559440E-05	1.627754E-04
8	C7	-9.152840E-05	-5.591400E-05	-5.531574E-05
9	H3	6.945647E-06	-4.233990E-05	5.958413E-05
10	H4	-2.806387E-06	-4.404424E-05	-1.146433E-05
11	H6	-3.174655E-05	2.933259E-05	-6.291090E-05
12	C16	-2.243026E-05	-2.386016E-04	-7.752165E-05
13	C8	1.235800E-04	1.062364E-04	2.216126E-05
14	N2	-4.252769E-05	4.913415E-04	-2.441794E-04
15	C9	-5.907516E-05	1.873556E-05	8.832746E-05
16	C10	7.121930E-06	2.225125E-04	-6.515139E-05
17	O1	-4.149598E-06	-3.484824E-04	1.488941E-04
18	C23	6.170585E-07	3.788789E-06	-6.965790E-06
19	C18	-1.489051E-04	5.292928E-05	-3.851714E-05
20	C19	-1.411750E-04	1.101775E-04	3.730492E-05
21	C20	-1.038763E-04	-2.739169E-04	-3.928527E-04
22	C21	-1.342634E-04	-6.719152E-05	-2.761956E-04
23	C22	1.189859E-04	3.630842E-06	2.672416E-05
24	H2	1.795638E-04	1.196113E-04	1.960139E-04
25	H5	-3.584733E-05	3.132857E-04	2.048779E-04
26	H7	5.872837E-05	8.128869E-05	8.895288E-06
27	H8	-1.098928E-05	1.012705E-04	2.095134E-04
28	H9	-2.611776E-05	6.477763E-05	1.852448E-05
29	H10	3.283739E-05	6.442765E-05	1.327011E-05
30	H19	-3.887030E-05	5.678065E-05	-9.916411E-06
31	H20	-3.024425E-05	3.151904E-05	1.158094E-05
32	H21	5.200948E-06	4.941005E-05	-5.337839E-05
33	H22	-6.166823E-05	6.321277E-05	-3.389977E-06

```
 34    H11    -1.536443E-04  -7.001633E-05  -3.172737E-05
 35    H12    -9.645787E-06  -1.447501E-04   5.151764E-05
 36    H13     1.930169E-05  -1.523432E-05  -1.481150E-05
-----------   -------------  -------------  -------------
   total      -7.408485E-04   1.101062E-03  -2.919993E-04

 end of program der1b


 start of program geopt  51

 geometry optimization step 51
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0108753
  Cos(theta):   0.7176881

  Final level shift:  -6.1241555E-02

 energy change:          -5.4772E-06 *  (  5.0000E-05 )
 gradient maximum:        8.5445E-04 .  (  4.5000E-04 )
 gradient rms:            1.6657E-04 *  (  3.0000E-04 )
 step size:   0.01088  trust radius:   0.01000
 displacement maximum:    5.9416E-03 .  (  1.8000E-03 )
 displacement rms:        9.8461E-04 *  (  1.2000E-03 )
 predicted energy change:    -1.0802E-05    geom step:   1.0875E-
02    full step:   1.0875E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -2.3402E-04     y:    -4.7577E-04     z:     1.8383E-04

 new geometry:
                                angstroms
 atom            x                 y                 z
 H1       -1.1777099107      1.8890016167     -2.2327163809
 C1       -1.0964684535      2.1213772258     -1.1844955086
 C2       -0.8846602999      2.6952777998      1.5038850430
 C3       -0.8778158937      1.0872713023     -0.2895851475
 C4       -1.2022245665      3.4355684428     -0.7600743067
 C5       -1.0969302741      3.7144647773      0.5902076144
 C6       -0.7673485674      1.3777817344      1.0723328211
 C7       -0.7862563358     -0.3523416086     -0.7568110028
 H3       -1.3672015948      4.2243142613     -1.4716317779
 H4       -1.1840463914      4.7266540862      0.9438188574
 H6       -0.8177509662      2.9330985547      2.5476270094
 C16       0.6135771135     -0.7649867223     -1.2100674828
```

```
  C8       -1.3983917335     -1.2495246395      0.3418372055
  N2       -0.5100390949      0.3378712618      1.9928933826
  C9       -0.7836880528     -0.9771835256      1.7047656910
  C10       0.0097724056      0.6531907553      3.3155893659
  O1       -0.5849373632     -1.8519954756      2.5005149750
  C23      -1.3884969161     -2.7412494098      0.0226318121
  C18       3.1415257953     -1.5837632955     -2.0936613789
  C19       0.7620309811     -1.4865147137     -2.3890905117
  C20       1.7594228772     -0.4496409767     -0.4853622505
  C21       3.0089432635     -0.8578821568     -0.9204463275
  C22       2.0119341033     -1.8948009600     -2.8292435145
  H2       -0.1079405649     -1.7344853504     -2.9718413402
  H5        1.6832532285      0.1251319827      0.4185460153
  H7        3.8803701918     -0.6046380716     -0.3430834276
  H8        2.0994951135     -2.4525134277     -3.7448653032
  H9        4.1136344684     -1.8977424511     -2.4308111241
  H10      -1.4319450544     -0.4528418178     -1.6227921390
  H19      -0.3788900907     -3.1284514624     -0.0235073180
  H20      -1.8687854997     -2.9188715379     -0.9350810627
  H21      -1.9220271978     -3.2929169891      0.7846984354
  H22      -2.4355103224     -0.9253117104      0.4389757902
  H11       0.8085749177      1.3790488490      3.2294289291
  H12       0.3901890531     -0.2537828334      3.7531069356
  H13      -0.7641986915      1.0542742079      3.9633166521

  nuclear repulsion energy.......  1414.932022180 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  51   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.334E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
```

```
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    326
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
70
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
143
  grid # 4      224    223    208    342    311    387    294
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    222    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    107    111   3729
  grid # 3      214    213    212    217   7186
  grid # 4      211    211    209    218   9912

  end of program grid


  start of program rwr
```

```
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                        RMS     maximum
      e  d  i  u  i                          energy  density   DIIS
      r  t  s  t  d     total energy        change  change    error

etot  1  N  N  1  U  -783.03312583751                  2.5E-05  1.4E-03
etot  2  Y  Y  4  M  -783.03323145682  1.1E-04  1.2E-05  5.5E-04
etot  3  Y  Y  4  M  -783.03324538246  1.4E-05  3.7E-06  1.4E-04
etot  4  Y  N  4  M  -783.03324892889  3.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.93202217953
   (E)  Total one-electron terms..... -3874.42734148806
   (I)  Total two-electron terms.....  1676.46207037964
   (L)  Electronic energy............. -2197.96527110842  (E+I)
   (N)  Total energy.................  -783.03324892889  (A+L)

 SCFE: SCF energy: HF    -783.03324892889 hartrees   iterations:
4


 HOMO energy:    -0.30214
 LUMO energy:     0.12931

  Orbital energies:
  -20.52665  -15.60062  -11.34624  -11.28621  -11.25666  -11.25009
  -11.24317  -11.24177  -11.24041  -11.23856  -11.23795  -11.23495
  -11.23109  -11.23042  -11.23001  -11.22943  -11.22838  -11.22764
  -11.20909   -1.39709   -1.26970   -1.16526   -1.14910   -1.10612
   -1.03016   -1.01875   -1.01803   -1.01277   -0.96257   -0.93282
   -0.85823   -0.83901   -0.83345   -0.82184   -0.79615   -0.74123
   -0.71106   -0.69509   -0.67286   -0.66438   -0.64468   -0.63760
   -0.62746   -0.61499   -0.61222   -0.60861   -0.59693   -0.58333
   -0.57646   -0.55352   -0.54887   -0.54065   -0.53092   -0.51902
   -0.51485   -0.50724   -0.50118   -0.49780   -0.48462   -0.46871
   -0.46292   -0.42161   -0.41156   -0.34271   -0.33288   -0.32308
   -0.30214    0.12931    0.13404    0.14444    0.15228    0.20377
    0.22972    0.24096    0.24890    0.26131    0.28801

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-2.482882E-05	5.177573E-05	-5.145735E-05
2	C1	-1.238259E-05	-4.214934E-05	5.559596E-05
3	C2	-9.689020E-06	-9.496388E-05	-2.001956E-05
4	C3	2.304038E-05	2.697201E-05	2.233112E-04
5	C4	-1.982807E-05	1.466823E-05	-3.183802E-05
6	C5	-2.217270E-05	3.377168E-05	-3.362130E-05
7	C6	-5.100440E-05	1.907202E-05	-2.233461E-04
8	C7	2.921073E-05	1.427224E-04	3.247637E-05
9	H3	-5.127241E-05	1.176837E-04	-8.651485E-05
10	H4	-3.711070E-05	1.098145E-04	-5.943565E-06
11	H6	-1.424875E-05	2.989317E-05	4.899068E-05
12	C16	-3.463249E-04	2.440185E-04	-1.123552E-05
13	C8	-8.198590E-05	-8.087593E-05	-9.865244E-06
14	N2	-6.021358E-05	-6.480846E-04	1.901373E-04
15	C9	-1.232772E-06	-2.109386E-04	2.674299E-04
16	C10	-2.332519E-04	-7.353139E-05	2.146582E-04
17	O1	-6.430481E-05	8.711837E-04	-5.324956E-04
18	C23	-4.455068E-05	2.291256E-05	-1.686378E-05
19	C18	4.388860E-04	4.287834E-05	1.411677E-04
20	C19	1.313401E-04	-1.348216E-04	-2.077970E-04
21	C20	3.591144E-04	2.500811E-04	2.980160E-04
22	C21	-7.149625E-05	1.697480E-04	2.927424E-04
23	C22	-5.413833E-04	-4.253767E-05	-2.638282E-04
24	H2	-4.289608E-04	-1.293857E-04	-3.827461E-04
25	H5	5.189263E-05	-9.527311E-06	1.758891E-04
26	H7	2.538659E-04	9.321166E-05	2.431716E-04
27	H8	-8.070462E-05	-9.926270E-05	-3.410422E-04
28	H9	4.972378E-05	-4.799946E-06	-1.659044E-05
29	H10	-7.687256E-05	-5.829530E-06	-3.842431E-05
30	H19	-1.694919E-05	8.143738E-06	-7.518820E-06
31	H20	-1.732300E-05	2.207636E-05	-2.550613E-05
32	H21	-4.303535E-05	1.502382E-05	1.896723E-05
33	H22	1.214811E-09	7.523111E-06	-5.420146E-06
34	H11	1.450811E-04	1.712002E-04	9.163344E-05
35	H12	-3.608523E-05	1.924162E-04	-5.779034E-05
36	H13	1.593889E-04	-5.739795E-05	-2.122706E-04
total		-7.456673E-04	1.022685E-03	-2.879480E-04

```
 end of program der1b
```

```
 start of program geopt  52

 geometry optimization step 52
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:           6.2080E-06 *  (  5.0000E-05 )
 gradient maximum:        9.6977E-04 .  (  4.5000E-04 )
 gradient rms:            2.4043E-04 *  (  3.0000E-04 )
 step size:   0.00855  trust radius:   0.01000
 displacement maximum:    4.3748E-03 .  (  1.8000E-03 )
 displacement rms:        7.7378E-04 *  (  1.2000E-03 )
 predicted energy change:    -6.5858E-06    geom step:   8.5467E-
03    full step:   8.5467E-03
 molecular structure not yet converged...

 center of mass moved by:
    x:     3.5033E-04     y:     1.9991E-04     z:    -2.2779E-04

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -1.1777087954     1.8883176899    -2.2327536475
 C1       -1.0969879317     2.1210581497    -1.1846428311
 C2       -0.8864913786     2.6957594783     1.5033300926
 C3       -0.8782195280     1.0872497486    -0.2894271431
 C4       -1.2034717513     3.4353611301    -0.7608782176
 C5       -1.0989008554     3.7146221518     0.5892922601
 C6       -0.7681777554     1.3781393300     1.0722690963
 C7       -0.7863716556    -0.3524022280    -0.7564508923
 H3       -1.3685691561     4.2237234090    -1.4727833082
 H4       -1.1866829506     4.7268525106     0.9425447145
 H6       -0.8203257149     2.9339978361     2.5469364891
 C16       0.6132987131    -0.7648804579    -1.2103499597
 C8       -1.3974910449    -1.2497579526     0.3427106021
 N2       -0.5100554865     0.3384594660     1.9930169453
 C9       -0.7818058224    -0.9763529334     1.7050162582
 C10       0.0096188319     0.6545958428     3.3156766230
 O1       -0.5800017569    -1.8501949242     2.4999361338
 C23      -1.3873699669    -2.7416276201     0.0240838481
 C18       3.1408397785    -1.5854500474    -2.0934858619
 C19       0.7614585694    -1.4823328532    -2.3924661498
 C20       1.7592098570    -0.4546196661    -0.4823501933
 C21       3.0085285298    -0.8638391489    -0.9171822057
 C22       2.0111607669    -1.8912800368    -2.8324879514
 H2       -0.1086018122    -1.7265071949    -2.9777886144
 H5        1.6833753189     0.1162819014     0.4245195416
```

```
  H7        3.8799715800     -0.6147882705     -0.3371685245
  H8        2.0985687358     -2.4455101569     -3.7505765597
  H9        4.1127372135     -1.9002569823     -2.4304255632
  H10      -1.4325773920     -0.4533962373     -1.6218538014
  H19      -0.3777644398     -3.1287720167     -0.0217863259
  H20      -1.8676100118     -2.9195334162     -0.9335630554
  H21      -1.9209878754     -3.2930536100      0.7862172232
  H22      -2.4345911738     -0.9259246358      0.4405277111
  H11       0.8070135769      1.3824140387      3.2297980135
  H12       0.3925704884     -0.2511004631      3.7530524316
  H13      -0.7648018972      1.0538274532      3.9628416471

  nuclear repulsion energy.......  1414.934410704 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  52   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.334E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     89     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
79
```

```
  grid # 3      223    223    207    194    174    211    176
145
  grid # 4      224    223    208    342    311    387    293
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    203    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    108    111   3730
  grid # 3      214    213    212    217   7190
  grid # 4      211    211    209    218   9910

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d    total energy      change  change    error

etot   1  N  N  1  U  -783.03321818875           1.7E-05  7.8E-04
etot   2  Y  Y  4  M  -783.03326062027  4.2E-05  7.5E-06  3.1E-04
```

```
etot   3  Y  Y  4  M  -783.03326964784  9.0E-06  2.4E-06  8.2E-05
etot   4  Y  N  4  M  -783.03326787528 -1.8E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.93441070356
   (E)  Total one-electron terms..... -3874.43985833599
   (I)  Total two-electron terms.....  1676.47217975715
   (L)  Electronic energy............. -2197.96767857884  (E+I)
   (N)  Total energy.................  -783.03326787528  (A+L)

 SCFE: SCF energy: HF    -783.03326787528 hartrees   iterations:
4


 HOMO energy:    -0.30206
 LUMO energy:     0.12931

  Orbital energies:
  -20.52685  -15.60016  -11.34578  -11.28588  -11.25653  -11.24986
  -11.24292  -11.24144  -11.24046  -11.23866  -11.23790  -11.23493
  -11.23135  -11.23054  -11.23011  -11.22966  -11.22860  -11.22764
  -11.20911   -1.39756   -1.26957   -1.16507   -1.14900   -1.10597
   -1.03004   -1.01868   -1.01788   -1.01270   -0.96256   -0.93272
   -0.85812   -0.83900   -0.83330   -0.82169   -0.79607   -0.74117
   -0.71095   -0.69500   -0.67285   -0.66433   -0.64465   -0.63754
   -0.62743   -0.61491   -0.61229   -0.60850   -0.59688   -0.58332
   -0.57630   -0.55344   -0.54881   -0.54066   -0.53098   -0.51903
   -0.51486   -0.50718   -0.50105   -0.49777   -0.48456   -0.46864
   -0.46284   -0.42156   -0.41147   -0.34260   -0.33293   -0.32290
   -0.30206    0.12931    0.13404    0.14451    0.15233    0.20411
    0.22975    0.24102    0.24896    0.26137    0.28828

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1     -3.114892E-05   2.389180E-05  -7.942389E-05
   2    C1     -3.396051E-05   3.754440E-05  -2.122494E-05
```

3	C2	-2.237622E-05	-4.412260E-05	-5.750733E-05
4	C3	7.705554E-06	-1.640225E-05	2.837941E-05
5	C4	-1.351911E-05	-3.598976E-05	-1.050528E-05
6	C5	-1.992820E-05	2.684687E-05	-4.751564E-06
7	C6	-1.149393E-05	5.921485E-05	-1.252274E-05
8	C7	7.866075E-05	1.992100E-05	8.417530E-05
9	H3	-3.417409E-05	9.563298E-05	-6.924522E-05
10	H4	-2.612069E-05	7.645631E-05	7.945233E-06
11	H6	6.664339E-06	1.899558E-05	1.048042E-04
12	C16	-1.116303E-04	1.060503E-04	-2.861163E-05
13	C8	-7.947596E-05	-2.778852E-05	-3.192787E-05
14	N2	5.964864E-05	2.154186E-04	2.522705E-04
15	C9	-1.255614E-04	8.614076E-05	-6.054017E-04
16	C10	1.548994E-04	1.134796E-04	-1.179084E-04
17	O1	7.121653E-06	-3.387642E-04	4.038366E-04
18	C23	-2.782810E-05	1.575454E-04	-3.626072E-05
19	C18	-1.841442E-05	3.660601E-05	9.173534E-06
20	C19	-1.758706E-06	1.343264E-05	3.115687E-05
21	C20	1.488126E-05	2.090122E-04	1.670951E-04
22	C21	3.061265E-05	3.766480E-05	-3.906252E-06
23	C22	-3.535025E-05	3.169778E-05	2.892352E-05
24	H2	-9.140491E-05	-3.659864E-05	-3.944124E-05
25	H5	-3.193586E-05	-6.318463E-05	-1.131711E-04
26	H7	-5.238995E-06	4.689703E-05	-1.261003E-05
27	H8	-1.625640E-05	-2.265168E-05	-7.828164E-05
28	H9	2.308281E-05	5.974614E-06	-3.881194E-05
29	H10	-9.532511E-05	1.522879E-05	-9.869114E-05
30	H19	2.619249E-05	1.259162E-05	-2.360470E-05
31	H20	-1.438520E-05	2.175129E-05	-3.940323E-05
32	H21	-3.594034E-05	5.405838E-06	3.655527E-05
33	H22	-5.189384E-05	4.147985E-05	-1.556094E-05
34	H11	-1.058360E-05	4.777469E-05	1.159852E-05
35	H12	-6.230350E-05	2.121973E-05	-3.782748E-05
36	H13	-1.414001E-04	8.538730E-05	1.008267E-04
total		-7.399392E-04	1.083760E-03	-3.098602E-04

end of program der1b

start of program geopt 53

geometry optimization step 53
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108
in five columns format

Level shifts adjusted to satisfy step-size constraints
Step size: 0.0142597
Cos(theta): 0.4320013

```
 Final level shift:  -8.4737900E-03

  energy change:          -1.8946E-05 *  (  5.0000E-05 )
  gradient maximum:        5.4724E-04 .  (  4.5000E-04 )
  gradient rms:            9.1960E-05 *  (  3.0000E-04 )
  step size:   0.01426  trust radius:   0.01414
  displacement maximum:    5.4362E-03 .  (  1.8000E-03 )
  displacement rms:        1.2910E-03 .  (  1.2000E-03 )
  predicted energy change:    -3.9909E-06    geom step:   1.4260E-
02    full step:   1.4260E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -6.6607E-05     y:     1.5252E-04     z:     8.9503E-05

  new geometry:
                                angstroms
  atom            x                 y                 z
  H1       -1.1823433758     1.8895725139     -2.2325604710
  C1       -1.0996111300     2.1217494272     -1.1841930638
  C2       -0.8841185643     2.6947732879      1.5042700518
  C3       -0.8778187320     1.0878178452     -0.2896606405
  C4       -1.2067290597     3.4356547888     -0.7591790898
  C5       -1.0994216843     3.7141985698      0.5912284777
  C6       -0.7658677868     1.3777892005      1.0720584509
  C7       -0.7856092226    -0.3513523222     -0.7574739731
  H3       -1.3744165704     4.2247521103     -1.4703670787
  H4       -1.1875870767     4.7263070622      0.9454616848
  H6       -0.8154074216     2.9316985000      2.5485298304
  C16       0.6143193631    -0.7634667555     -1.2106960751
  C8       -1.3984518843    -1.2488983903      0.3405767170
  N2       -0.5065062264     0.3377204733      1.9919382335
  C9       -0.7834489078    -0.9763255849      1.7031653465
  C10       0.0114916218     0.6549494331      3.3147771050
  O1       -0.5857159785    -1.8498863750      2.5003638764
  C23      -1.3879132193    -2.7403179538      0.0210868375
  C18       3.1415839344    -1.5874782971     -2.0915862461
  C19       0.7620981600    -1.4851797946     -2.3900315066
  C20       1.7603396540    -0.4512261465     -0.4839557576
  C21       3.0095776302    -0.8624417602     -0.9177812545
  C22       2.0118857694    -1.8952832994     -2.8290995858
  H2       -0.1084622864    -1.7329148310     -2.9736232943
  H5        1.6839648901     0.1206767168      0.4213223507
  H7        3.8811032514    -0.6119897058     -0.3388652748
  H8        2.0990070956    -2.4525426768     -3.7454630940
  H9        4.1134549466    -1.9040624626     -2.4278652728
  H10      -1.4314004101    -0.4518498346     -1.6239666563
  H19      -0.3782589120    -3.1272987803     -0.0248091216
  H20      -1.8672394378    -2.9184583587     -0.9367914773
  H21      -1.9212516765    -3.2922826175      0.7831437284
  H22      -2.4354452974    -0.9242211372      0.4374168624
```

```
  H11       0.8057525327      1.3866673184      3.2304126811
  H12       0.3970374473     -0.2506582098      3.7492502888
  H13      -0.7645367465      1.0499818635      3.9646101221

  nuclear repulsion energy.......  1414.940729313 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  53   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.336E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     83
81
  grid # 2      116     97     96     98     97     97     95
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    324
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
145
  grid # 4      224    223    208    342    311    387    293
274

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
```

```
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     66     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    222    223    224    202    218    216
217
  grid # 4      207    223    224    224    197    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2863
  grid # 2      110    109    108    111   3731
  grid # 3      214    213    212    217   7186
  grid # 4      211    211    209    218   9912

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS     maximum
       t  p  i  c  r                                      density    DIIS
       e  d  i  u  i                        energy        change     error
       r  t  s  t  d     total energy       change

etot   1  N  N  1  U  -783.03317801295                    1.9E-05   5.2E-04
etot   2  Y  Y  4  M  -783.03322410261   4.6E-05          7.6E-06   2.1E-04
etot   3  Y  Y  4  M  -783.03323026551   6.2E-06          2.0E-06   5.2E-05
etot   4  Y  N  4  M  -783.03323331725   3.1E-06          0.0E+00   0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.94072931277
   (E)  Total one-electron terms..... -3874.44892683825
   (I)  Total two-electron terms.....  1676.47496420823
```

```
   (L)  Electronic energy..... -2197.97396263002  (E+I)
   (N)  Total energy.................  -783.03323331725  (A+L)

 SCFE: SCF energy: HF    -783.03323331725 hartrees   iterations:
4


 HOMO energy:    -0.30207
 LUMO energy:     0.12934

  Orbital energies:
 -20.52679  -15.60041  -11.34609  -11.28582  -11.25677  -11.25002
 -11.24318  -11.24157  -11.24048  -11.23870  -11.23799  -11.23493
 -11.23127  -11.23051  -11.23016  -11.22964  -11.22850  -11.22761
 -11.20911   -1.39722   -1.26958   -1.16514   -1.14899   -1.10611
  -1.03012   -1.01865   -1.01795   -1.01268   -0.96261   -0.93276
  -0.85820   -0.83891   -0.83339   -0.82171   -0.79608   -0.74114
  -0.71103   -0.69503   -0.67280   -0.66431   -0.64465   -0.63750
  -0.62741   -0.61492   -0.61213   -0.60849   -0.59705   -0.58330
  -0.57639   -0.55349   -0.54870   -0.54069   -0.53087   -0.51919
  -0.51482   -0.50723   -0.50110   -0.49775   -0.48458   -0.46866
  -0.46291   -0.42149   -0.41165   -0.34259   -0.33290   -0.32301
  -0.30207    0.12934    0.13403    0.14444    0.15231    0.20368
   0.22963    0.24095    0.24898    0.26123    0.28810

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1      2.009787E-06   5.513706E-05   1.351264E-04
   2    C1      1.321892E-05  -2.250161E-07   3.721129E-05
   3    C2     -4.197925E-05   3.170594E-04   1.548409E-04
   4    C3     -8.108976E-05   7.273175E-05  -1.436090E-04
   5    C4     -2.845503E-05   2.426566E-04   2.839050E-05
   6    C5     -2.964024E-05   3.832562E-05  -2.597070E-05
   7    C6     -4.244912E-05   3.620935E-05  -1.346349E-04
   8    C7     -2.369886E-04   1.299283E-04  -2.853163E-04
   9    H3      2.843962E-05  -1.408228E-04   1.473250E-04
  10    H4     -2.355475E-06  -6.907360E-05  -6.455204E-05
```

```
 11    H6     -1.152681E-04   7.450662E-05  -3.178092E-04
 12    C16    -1.969633E-04  -1.403705E-04   1.159929E-04
 13    C8      1.680767E-04   2.015960E-04  -1.238589E-04
 14    N2     -4.051292E-04   4.978379E-04  -5.912989E-04
 15    C9      3.362542E-04  -2.691790E-04   1.244593E-03
 16    C10    -3.466211E-04  -7.444472E-05   3.235407E-04
 17    O1     -1.596396E-04   2.421969E-04  -6.005190E-04
 18    C23    -4.808766E-06  -1.656182E-04   1.874576E-04
 19    C18     3.700599E-04  -8.696416E-05  -1.544217E-04
 20    C19    -8.574665E-07  -1.295772E-04  -2.939109E-04
 21    C20     1.291058E-04  -1.863535E-04  -2.056099E-04
 22    C21    -1.689381E-04   3.119957E-04   3.146566E-04
 23    C22    -4.422643E-04  -1.174591E-04  -2.810819E-04
 24    H2      1.040526E-04   1.151951E-04  -4.145322E-06
 25    H5      5.243907E-05   2.760510E-04   3.221320E-04
 26    H7      9.570046E-05   5.602606E-05   1.235507E-04
 27    H8     -2.695225E-05   7.047751E-06  -6.057148E-05
 28    H9     -1.397125E-04   9.994178E-05   3.479694E-05
 29    H10     1.445351E-04   6.103886E-05   2.145055E-04
 30    H19     4.313937E-05   4.473298E-05   2.520898E-05
 31    H20    -1.453667E-04   6.456276E-05  -9.771683E-05
 32    H21    -5.606348E-05   2.288666E-05  -3.837125E-05
 33    H22    -1.616229E-06  -4.163522E-05   1.382352E-05
 34    H11    -6.985654E-05  -2.270576E-04  -6.385733E-05
 35    H12     2.276885E-04  -5.867645E-05   3.232349E-04
 36    H13     2.838489E-04  -2.120761E-04  -5.258176E-04
-----------   -------------  -------------  -------------
   total      -7.444461E-04   1.048131E-03  -2.666858E-04

 end of program der1b


 start of program geopt  54

 geometry optimization step 54
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 ** restarting optimization from step   53 **


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0107981
  Cos(theta):   0.5061370

  Final level shift:  -1.9838567E-02

 energy change:           3.4558E-05 *  (  5.0000E-05 )
 gradient maximum:        5.4724E-04 .  (  4.5000E-04 )
 gradient rms:            9.1960E-05 *  (  3.0000E-04 )
 step size:   0.01080  trust radius:   0.01000
```

```
  displacement maximum:    5.5467E-03 .  (  1.8000E-03 )
  displacement rms:        9.7761E-04 *  (  1.2000E-03 )
  predicted energy change:    -3.9323E-06    geom step:   1.0798E-
02    full step:   1.0798E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -7.6328E-17     y:     2.7062E-16     z:     1.3878E-16

  new geometry:
                                 angstroms
  atom           x                  y                  z
  H1       -1.1808884946      1.8897821389     -2.2322586386
  C1       -1.0989064553      2.1219773734     -1.1839158930
  C2       -0.8853652790      2.6952373354      1.5044089141
  C3       -0.8780731966      1.0880024937     -0.2891918639
  C4       -1.2060067519      3.4359682404     -0.7594038837
  C5       -1.0997580361      3.7145665621      0.5910542372
  C6       -0.7668530693      1.3780327796      1.0725235878
  C7       -0.7857896461     -0.3510750743     -0.7573867601
  H3       -1.3729599797      4.2248483092     -1.4708586162
  H4       -1.1879593799      4.7267688649      0.9449260270
  H6       -0.8177581902      2.9326123541      2.5484150014
  C16       0.6140947597     -0.7630823130     -1.2108160782
  C8       -1.3980823017     -1.2490640930      0.3406932522
  N2       -0.5082455406      0.3377595873      1.9927758317
  C9       -0.7823455573     -0.9766991427      1.7032157695
  C10       0.0113457667      0.6544420130      3.3153783738
  O1       -0.5828462117     -1.8507322937      2.4992176106
  C23      -1.3880279559     -2.7405836558      0.0212107094
  C18       3.1415356867     -1.5870115396     -2.0918299927
  C19       0.7620892697     -1.4852388318     -2.3900542734
  C20       1.7600668918     -0.4504122182     -0.4841794631
  C21       3.0094291402     -0.8614878589     -0.9180017716
  C22       2.0117985612     -1.8953977474     -2.8292548894
  H2       -0.1083386741     -1.7335533775     -2.9734061005
  H5        1.6836645145      0.1207813161      0.4211660164
  H7        3.8807379818     -0.6110941617     -0.3391902702
  H8        2.0991162346     -2.4528170503     -3.7456428533
  H9        4.1132261799     -1.9034837478     -2.4283197648
  H10      -1.4317235397     -0.4517251668     -1.6234495507
  H19      -0.3784263081     -3.1277243751     -0.0254555717
  H20      -1.8684461124     -2.9182163081     -0.9363596389
  H21      -1.9211834427     -3.2925384779      0.7834406304
  H22      -2.4351319781     -0.9248252527      0.4382080597
  H11       0.8094041423      1.3818416781      3.2296827518
  H12       0.3927840267     -0.2514783633      3.7527387889
  H13      -0.7633912560      1.0546993235      3.9632691161

  nuclear repulsion energy.......  1414.891375649 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  54   /
```

```
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.335E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
79
  grid # 3      223    223    207    194    174    211    176
145
  grid # 4      224    223    208    342    311    387    293
275

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     80     97     95     96     97     96
112
  grid # 3      257    150    183    183    182    184    183
212
  grid # 4      450    285    327    326    327    327    327
211
```

```
  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
  grid # 3      212    223    223    224    202    218    216
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2865
  grid # 2      110    109    108    111   3730
  grid # 3      214    213    212    217   7188
  grid # 4      211    211    209    218   9910

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                                 energy density   DIIS
       e  d  i  u  i                  total energy   change change    error

etot   1  N  N  1  U  -783.03324514701                1.3E-05  2.7E-04
etot   2  Y  Y  4  M  -783.03325823767  1.3E-05       4.1E-06  6.9E-05
etot   3  Y  N  4  M  -783.03325972614  1.5E-06       0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.89137564935
   (E)  Total one-electron terms..... -3874.35225017420
   (I)  Total two-electron terms.....  1676.42761479872
   (L)  Electronic energy............. -2197.92463537548  (E+I)
   (N)  Total energy.................  -783.03325972614  (A+L)

 SCFE: SCF energy: HF    -783.03325972614 hartrees   iterations:
3


 HOMO energy:    -0.30209
 LUMO energy:     0.12934
```

Orbital energies:

-20.52685	-15.60029	-11.34601	-11.28585	-11.25673	-11.25001
-11.24311	-11.24158	-11.24050	-11.23869	-11.23799	-11.23492
-11.23127	-11.23050	-11.23016	-11.22964	-11.22849	-11.22765
-11.20914	-1.39727	-1.26944	-1.16510	-1.14897	-1.10603
-1.03008	-1.01865	-1.01788	-1.01270	-0.96255	-0.93275
-0.85813	-0.83889	-0.83337	-0.82173	-0.79607	-0.74110
-0.71099	-0.69502	-0.67282	-0.66429	-0.64457	-0.63754
-0.62743	-0.61488	-0.61217	-0.60853	-0.59695	-0.58333
-0.57637	-0.55347	-0.54875	-0.54065	-0.53094	-0.51911
-0.51484	-0.50721	-0.50105	-0.49775	-0.48459	-0.46866
-0.46291	-0.42148	-0.41157	-0.34258	-0.33287	-0.32297
-0.30209	0.12934	0.13404	0.14442	0.15229	0.20386
0.22969	0.24097	0.24889	0.26136	0.28827	

end of program scf

start of program der1a
end of program der1a

start of program rwr
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	-1.557846E-05	1.909331E-05	8.792398E-05
2	C1	-6.615045E-06	-5.113308E-06	-7.490206E-06
3	C2	-2.163787E-05	2.170730E-04	2.440879E-05
4	C3	-4.803961E-05	6.059738E-05	-2.105484E-04
5	C4	-3.758897E-05	1.588430E-04	1.109556E-04
6	C5	-2.375369E-05	5.111599E-05	-4.973671E-05
7	C6	-3.384572E-05	-3.947816E-05	1.519769E-05
8	C7	-1.725157E-04	1.046236E-05	-1.162194E-04
9	H3	5.832331E-06	-9.250547E-05	1.177743E-04
10	H4	-7.571445E-06	-6.435223E-05	-2.494453E-05
11	H6	-3.706344E-05	5.458788E-05	-1.335005E-04
12	C16	-1.084880E-04	-1.784527E-04	1.824923E-05
13	C8	1.633554E-04	1.375414E-04	1.550168E-05
14	N2	-9.861134E-05	3.722121E-04	-4.499002E-04
15	C9	6.635431E-05	-1.471067E-04	7.969503E-04
16	C10	-4.239099E-04	2.081977E-04	1.607719E-04
17	O1	-1.238035E-04	1.390459E-04	-3.526588E-04
18	C23	-3.225745E-05	-2.422860E-05	4.198379E-05
19	C18	1.914918E-04	4.791890E-05	-8.209416E-06

```
  20    C19    -5.629705E-05  -8.353819E-05  -1.946208E-04
  21    C20     2.129825E-04  -4.153653E-04  -4.358897E-04
  22    C21    -3.440109E-04   1.067036E-04   1.542453E-05
  23    C22    -3.277768E-04  -3.603680E-05  -1.960225E-04
  24    H2      1.812240E-05   1.199201E-04  -3.360019E-05
  25    H5      2.770088E-05   4.607813E-04   4.940732E-04
  26    H7      2.445453E-04   1.115868E-04   2.099182E-04
  27    H8     -6.022483E-05   3.551908E-05   3.116587E-05
  28    H9     -3.287708E-05   8.013944E-05   5.279441E-05
  29    H10     5.806747E-05   8.002471E-05   6.885619E-05
  30    H19     2.788493E-05   2.928524E-05   1.200502E-05
  31    H20    -6.551069E-05   4.254804E-05  -5.127353E-05
  32    H21    -1.826397E-05   3.952308E-05  -2.778255E-05
  33    H22     7.891052E-06   2.638067E-05   1.099637E-05
  34    H11    -1.240271E-04  -7.498921E-05  -2.730063E-05
  35    H12     1.387464E-04  -1.691782E-04   1.305933E-04
  36    H13     3.060384E-04  -1.919730E-04  -3.754518E-04
 -----------   -------------  -------------  -------------
    total      -7.512553E-04   1.086783E-03  -2.796055E-04

  end of program der1b


  start of program geopt  55

  geometry optimization step 55
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  ** restarting optimization from step   53 **


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0105038
   Cos(theta):   0.4758084

   Final level shift:  -1.5642341E-02

  energy change:           8.1491E-06 *  (  5.0000E-05 )
  gradient maximum:        5.4724E-04 .  (  4.5000E-04 )
  gradient rms:            9.1960E-05 *  (  3.0000E-04 )
  step size:   0.01050  trust radius:   0.01000
  displacement maximum:    5.8157E-03 .  (  1.8000E-03 )
  displacement rms:        9.5097E-04 *  (  1.2000E-03 )
  predicted energy change:    -3.4011E-06    geom step:   1.0504E-
02    full step:   1.0504E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.4572E-16     y:    -1.0963E-15     z:     8.3267E-17
```

```
 new geometry:
                                angstroms
 atom            x                   y                   z
 H1       -1.1799100718      1.8898995885     -2.2322329625
 C1       -1.0983163375      2.1220312076     -1.1839185242
 C2       -0.8857155668      2.6953496590      1.5044014209
 C3       -0.8782353531      1.0879491939     -0.2891989199
 C4       -1.2050970136      3.4360582873     -0.7594886488
 C5       -1.0993776441      3.7146594757      0.5909437708
 C6       -0.7674092348      1.3780413884      1.0725755577
 C7       -0.7859911141     -0.3512185128     -0.7572882358
 H3       -1.3713536947      4.2248674483     -1.4709800974
 H4       -1.1873571163      4.7268667324      0.9446667904
 H6       -0.8186388885      2.9328864171      2.5482426649
 C16       0.6138983530     -0.7634172563     -1.2105702538
 C8       -1.3981840927     -1.2491829274      0.3408635973
 N2       -0.5090644922      0.3376940663      1.9928825053
 C9       -0.7825778951     -0.9770650176      1.7036163486
 C10       0.0115272626      0.6536514328      3.3152192128
 O1       -0.5832412670     -1.8516418014      2.4991247915
 C23      -1.3885265446     -2.7408219174      0.0214822387
 C18       3.1415791620     -1.5861906626     -2.0919890740
 C19       0.7621666278     -1.4859347804     -2.3894551978
 C20       1.7597732805     -0.4497120230     -0.4845303191
 C21       3.0092489734     -0.8600881083     -0.9185335773
 C22       2.0119030521     -1.8957108546     -2.8288204330
 H2       -0.1080084481     -1.7344093552     -2.9725890454
 H5        1.6834093239      0.1223444677      0.4203230613
 H7        3.8804601471     -0.6088749823     -0.3401834708
 H8        2.0994190190     -2.4535406399     -3.7448086728
 H9        4.1133186819     -1.9020349436     -2.4286168057
 H10      -1.4317539531     -0.4518571669     -1.6232613724
 H19      -0.3789538018     -3.1282056898     -0.0250513646
 H20      -1.8690994697     -2.9181393258     -0.9361711511
 H21      -1.9220610200     -3.2925991781      0.7835859122
 H22      -2.4352688833     -0.9250718290      0.4384740446
 H11       0.8104470787      1.3803578737      3.2284492921
 H12       0.3929253844     -0.2527750502      3.7533838518
 H13      -0.7631486517      1.0549141051      3.9628018827

 nuclear repulsion energy.......  1414.880671647 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  55   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.335E-04
 number of canonical orbitals.....          368
 end of program onee
```

```
  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       72     87     89     90     89     88     84
81
  grid # 2      116     97     96     98     97     97     94
90
  grid # 3      217    182    184    194    183    184    189
177
  grid # 4      216    326    328    338    328    328    323
314

  number of gridpoints:
     atom        H3     H4     H6    C16     C8     N2     C9
C10
  grid # 1       73     73     70     92     82     95     82
69
  grid # 2      118    118    112    100     90    105     92
80
  grid # 3      223    223    207    194    174    211    176
144
  grid # 4      224    223    208    342    311    387    293
273

  number of gridpoints:
     atom        O1    C23    C18    C19    C20    C21    C22
H2
  grid # 1      111     74     89     88     88     89     89
71
  grid # 2      123     79     97     95     96     97     96
112
  grid # 3      257    149    183    183    182    184    183
212
  grid # 4      450    286    327    326    327    327    327
211

  number of gridpoints:
     atom        H5     H7     H8     H9    H10    H19    H20
H21
  grid # 1       71     73     73     73     67     71     71
70
  grid # 2      111    118    118    118    106    108    110
108
```

```
  grid # 3      212    222    223    224    202    218    217
217
  grid # 4      207    223    224    224    196    212    216
215

  number of gridpoints:
     atom       H22    H11    H12    H13  total
  grid # 1       69     71     70     71   2865
  grid # 2      110    109    108    111   3730
  grid # 3      214    213    212    217   7186
  grid # 4      211    211    209    218   9909

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03325921999           6.4E-06  1.3E-04
etot   2  Y  Y  4  M  -783.03326131730  2.1E-06  2.2E-06  5.6E-05
etot   3  Y  N  4  M  -783.03326233200  1.0E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1414.88067164681
   (E)  Total one-electron terms..... -3874.33130696955
   (I)  Total two-electron terms.....  1676.41737299074
   (L)  Electronic energy............. -2197.91393397881  (E+I)
   (N)  Total energy.................  -783.03326233200  (A+L)

 SCFE: SCF energy: HF    -783.03326233200 hartrees   iterations:
3


 HOMO energy:    -0.30211
 LUMO energy:     0.12934

  Orbital energies:
  -20.52693  -15.60025  -11.34597  -11.28589  -11.25678  -11.24998
  -11.24305  -11.24158  -11.24049  -11.23871  -11.23800  -11.23494
  -11.23126  -11.23049  -11.23018  -11.22960  -11.22849  -11.22761
  -11.20915   -1.39721   -1.26942   -1.16512   -1.14901   -1.10601
   -1.03007   -1.01867   -1.01790   -1.01273   -0.96242   -0.93275
   -0.85809   -0.83889   -0.83338   -0.82177   -0.79608   -0.74111
```

```
 -0.71097   -0.69504   -0.67282   -0.66431   -0.64454   -0.63755
 -0.62744   -0.61491   -0.61219   -0.60855   -0.59687   -0.58335
 -0.57638   -0.55343   -0.54874   -0.54061   -0.53093   -0.51903
 -0.51485   -0.50720   -0.50107   -0.49776   -0.48460   -0.46866
 -0.46290   -0.42148   -0.41152   -0.34262   -0.33287   -0.32299
 -0.30211    0.12934    0.13404    0.14442    0.15228    0.20391
  0.22971    0.24096    0.24885    0.26138    0.28823

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H1     -1.749000E-05   8.711360E-06   3.667251E-05
  2    C1     -1.645016E-05   1.144735E-05  -2.636625E-05
  3    C2     -3.000772E-05   1.123093E-04  -5.008545E-05
  4    C3     -1.411692E-05   3.177434E-05  -1.192363E-04
  5    C4     -3.279182E-05   8.437073E-05   1.137831E-04
  6    C5     -2.457905E-05   5.395061E-05  -6.651527E-05
  7    C6      3.413228E-06  -7.756193E-05   4.479291E-05
  8    C7     -8.703170E-05  -1.700346E-05  -8.896058E-06
  9    H3     -1.542373E-05  -2.381602E-05   5.475093E-05
 10    H4     -1.726452E-05  -2.658623E-05  -1.229626E-06
 11    H6     -8.399232E-06   4.335350E-05   5.450883E-07
 12    C16    -1.518763E-04  -7.777962E-05  -3.681900E-05
 13    C8      7.995412E-05   3.687085E-05   8.798725E-05
 14    N2     -2.350112E-06  -7.172780E-05  -2.459148E-04
 15    C9     -9.171887E-05  -1.461367E-04   4.503970E-04
 16    C10    -2.248068E-04   1.945003E-04   3.383153E-04
 17    O1     -2.382327E-05   4.053541E-04  -3.348692E-04
 18    C23    -2.778282E-05   3.300922E-05  -4.729064E-05
 19    C18     1.891842E-04   9.526208E-05   8.908498E-05
 20    C19     5.600796E-06  -5.576541E-05  -1.784688E-04
 21    C20     2.987256E-04  -3.277978E-04  -3.353849E-04
 22    C21    -3.442854E-04   2.298487E-05  -4.611124E-05
 23    C22    -3.502592E-04   4.481850E-07  -1.666977E-04
 24    H2     -1.570598E-04   3.829258E-05  -1.436904E-04
 25    H5      1.961258E-05   4.217267E-04   5.015034E-04
 26    H7      3.277167E-04   1.393539E-04   2.737490E-04
 27    H8     -8.260342E-05   3.942657E-06  -4.727012E-05
```

28	H9	3.165801E-05	4.776196E-05	4.444761E-05
29	H10	-2.445490E-05	6.095446E-05	-1.796525E-05
30	H19	-2.530227E-05	2.836178E-05	-1.433523E-06
31	H20	-1.228766E-05	2.885540E-05	-3.720262E-06
32	H21	6.855388E-06	5.299271E-05	-2.404386E-05
33	H22	7.386567E-06	5.527752E-05	3.405201E-06
34	H11	-2.645177E-04	-1.473943E-04	9.281596E-05
35	H12	-1.393942E-04	2.427787E-04	-1.598089E-04
36	H13	4.827509E-04	-2.027214E-04	-3.397871E-04
total		-7.332195E-04	1.080355E-03	-2.693544E-04

end of program der1b

start of program geopt 56

geometry optimization step 56
** stopping now - optimization seems to be stuck **

****
** Geometry optimization complete **
****

center of mass moved by:
x: 0.0000E+00 y: 0.0000E+00 z: 0.0000E+00

final geometry:

		angstroms	
atom	x	y	z
H1	-1.1799100718	1.8898995885	-2.2322329625
C1	-1.0983163375	2.1220312076	-1.1839185242
C2	-0.8857155668	2.6953496590	1.5044014209
C3	-0.8782353531	1.0879491939	-0.2891989199
C4	-1.2050970136	3.4360582873	-0.7594886488
C5	-1.0993776441	3.7146594757	0.5909437708
C6	-0.7674092348	1.3780413884	1.0725755577
C7	-0.7859911141	-0.3512185128	-0.7572882358
H3	-1.3713536947	4.2248674483	-1.4709800974
H4	-1.1873571163	4.7268667324	0.9446667904
H6	-0.8186388885	2.9328864171	2.5482426649
C16	0.6138983530	-0.7634172563	-1.2105702538
C8	-1.3981840927	-1.2491829274	0.3408635973
N2	-0.5090644922	0.3376940663	1.9928825053
C9	-0.7825778951	-0.9770650176	1.7036163486
C10	0.0115272626	0.6536514328	3.3152192128
O1	-0.5832412670	-1.8516418014	2.4991247915
C23	-1.3885265446	-2.7408219174	0.0214822387
C18	3.1415791620	-1.5861906626	-2.0919890740
C19	0.7621666278	-1.4859347804	-2.3894551978
C20	1.7597732805	-0.4497120230	-0.4845303191

```
 C21       3.0092489734     -0.8600881083     -0.9185335773
 C22       2.0119030521     -1.8957108546     -2.8288204330
 H2       -0.1080084481     -1.7344093552     -2.9725890454
 H5        1.6834093239      0.1223444677      0.4203230613
 H7        3.8804601471     -0.6088749823     -0.3401834708
 H8        2.0994190190     -2.4535406399     -3.7448086728
 H9        4.1133186819     -1.9020349436     -2.4286168057
 H10      -1.4317539531     -0.4518571669     -1.6232613724
 H19      -0.3789538018     -3.1282056898     -0.0250513646
 H20      -1.8690994697     -2.9181393258     -0.9361711511
 H21      -1.9220610200     -3.2925991781      0.7835859122
 H22      -2.4352688833     -0.9250718290      0.4384740446
 H11       0.8104470787      1.3803578737      3.2284492921
 H12       0.3929253844     -0.2527750502      3.7533838518
 H13      -0.7631486517      1.0549141051      3.9628018827

 nuclear repulsion energy.......  1414.880671647 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  56   /
------------------------------------------------

 end of program geopt


 start of program post
 Writing a SPARTAN archive file
 end of program post

Total cpu seconds     user:    3923.109   user+sys:    3923.109
```

CIS 2 (PH_EQ – ME_AX)

```
+-----------------------------------------------------------------
---+
  |  Jaguar version 3.5, release  42
|
  |
|
  |  Copyright 1991-1998 Schrodinger, Inc.
|
  |  All Rights Reserved.
|
  |
|
  |  Use of this program should be acknowledged in publications
as:    |
  |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.
|
  +-----------------------------------------------------------------
-----+

  start of program pre
  Job name: WF29000
  Executables used: D:\TITAN
  Temporary files : C:\Users\gfabr\AppData\Local\Temp\WF29000

  Input file comments:
    Molecule001
    This file created by Spartan

  basis set:             6-31G**
  net molecular charge:    0
  multiplicity:            1

  number of basis functions....          370

 Input geometry:
                                 angstroms
  atom            x                  y                  z
  H1       -0.1057860000      1.2372270000     -2.1093050000
  C1       -0.0774240000      1.7068310000     -1.1175650000
  C2        0.0087040000      2.9151390000      1.3846380000
  C3        0.2607620000      0.9372920000     -0.0057490000
  C4       -0.3782970000      3.0571860000     -0.9878350000
  C5       -0.3455530000      3.6562940000      0.2650770000
  C6        0.3324840000      1.5574230000      1.2576320000
  C7        0.6189860000     -0.5157620000     -0.1363140000
  H3       -0.6426930000      3.6449960000     -1.8726740000
  H4       -0.5961860000      4.7167940000      0.3731070000
  H6        0.0290920000      3.4098080000      2.3636220000
  H7        1.7409960000     -0.5338270000     -0.1838720000
  C10       0.1103230000     -1.2048020000     -1.3745680000
```

```
  C8        0.2067290000     -1.3009890000      1.1228110000
  C17      -1.2938690000     -1.4425820000      1.3172120000
  N2        0.7183370000      0.8050980000      2.4281180000
  C9        0.8036850000     -0.6169380000      2.3464920000
  C16       1.4234250000      1.5370750000      3.5045810000
  O1        1.3001730000     -1.2312870000      3.2789440000
  C11      -0.7655750000     -2.5633220000     -3.6565150000
  C12       0.9837500000     -2.0329400000     -2.0855370000
  C13      -1.2057310000     -1.0644300000     -1.8202950000
  C14      -1.6399100000     -1.7403290000     -2.9551680000
  C15       0.5467140000     -2.7078020000     -3.2195810000
  H19       2.0203760000     -2.1543720000     -1.7485610000
  H20      -1.8973790000     -0.4123760000     -1.2713980000
  H21      -2.6741570000     -1.6229390000     -3.2953130000
  H22       1.2388710000     -3.3545650000     -3.7688460000
  H23      -1.1089860000     -3.0954060000     -4.5495090000
  H27      -1.8057990000     -0.4707090000      1.3005120000
  H29      -1.7350530000     -2.0581730000      0.5209810000
  H30       0.6441890000     -2.3278130000      1.0421280000
  H15      -1.5241950000     -1.9275430000      2.2746670000
  H2        2.0644920000      2.3308300000      3.0949130000
  H5        2.0560900000      0.8683330000      4.1042560000
  H8        0.6884140000      1.9985800000      4.1789160000

  Molecular weight:    251.13 amu

  Stoichiometry:        C17NH17O
  Molecular Point Group: C1
  Point Group used: C1
  nuclear repulsion energy.......  1394.502457810 hartrees

 Non-default options chosen:
   Geometry will be optimized in redundant internal coordinates
   Initial Hessian: from previous calculation

  end of program pre


  start of program onee
  smallest eigenvalue of S:    3.549E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program hfig
  initial wavefunction generated automatically from atomic
wavefunctions

  Irreducible     Total no   No of occupied orbitals
  representation  orbitals   Shell_1  Shell_2    ...
  No Symm          368         67
  ------------------------
```

```
  Orbital occupation/shell    1.000

  end of program hfig


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     88     88     89     89     86
81
  grid # 2      114     96     95     98     97     97     96
90
  grid # 3      211    184    184    192    184    185    189
175
  grid # 4      217    327    328    337    327    327    327
309

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     69     92     82     72
98
  grid # 2      118    118    113    109    100     91     79
105
  grid # 3      224    223    209    213    196    175    153
215
  grid # 4      232    232    217    208    341    310    296
393

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       86     73    111     89     87     87     88
89
  grid # 2       94     80    122     97     95     95     95
97
  grid # 3      178    149    262    185    184    182    183
185
  grid # 4      298    280    459    327    328    326    326
327

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     70
69
```

```
  grid # 2      113    111    118    118    118    108    109
111
  grid # 3      214    210    224    224    224    214    209
215
  grid # 4      222    214    232    232    232    215    212
216

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2873
  grid # 2      111    110    110    110   3738
  grid # 3      219    215    215    217   7220
  grid # 4      225    221    222    222  10064

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf
 number of electrons.........        134
 number of alpha electrons....         67
 number of beta electrons.....         67
 number of orbitals, total....        368
 number of core orbitals......         67
 number of open shell orbs....          0
 number of occupied orbitals..         67
 number of virtual orbitals...        301
 number of hamiltonians.......          1
 number of shells.............          1
 SCF type: HF

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                                 energy density   DIIS
       e  d  i  u  i                 total energy    change change    error

etot   1  N  N  5  M  -780.39716462191                4.5E-03  1.0E-01
etot   2  Y  Y  6  M  -782.67604398440  2.3E+00       2.0E-03  4.2E-02
etot   3  Y  Y  6  M  -782.93083475678  2.5E-01       8.9E-04  2.6E-02
etot   4  N  Y  2  U  -782.99815335980  6.7E-02       6.0E-04  1.2E-02
etot   5  Y  Y  6  M  -783.00797122904  9.8E-03       9.4E-04  6.9E-03
etot   6  N  Y  2  U  -783.01277668103  4.8E-03       1.0E-04  1.6E-03
etot   7  Y  Y  6  M  -783.01303150056  2.5E-04       4.0E-05  4.3E-04
etot   8  Y  Y  6  M  -783.01308149635  5.0E-05       1.1E-05  1.5E-04
etot   9  Y  Y  6  M  -783.01309224379  1.1E-05       4.8E-06  4.9E-05
etot  10  Y  N  6  M  -783.01309985574  7.6E-06       0.0E+00  0.0E+00


 Energy components, in hartrees:
```

```
   (A)  Nuclear repulsion.....  1394.50245781033
   (E)  Total one-electron terms..... -3833.55266757138
   (I)  Total two-electron terms.....  1656.03710990532
   (L)  Electronic energy..... -2177.51555766607  (E+I)
   (N)  Total energy.............  -783.01309985574  (A+L)

 SCFE: SCF energy: HF    -783.01309985574 hartrees   iterations:
10


 HOMO energy:    -0.30079
 LUMO energy:     0.12588

  Orbital energies:
 -20.52986  -15.60154  -11.35514  -11.28848  -11.26329  -11.25408
 -11.25208  -11.24667  -11.24510  -11.24177  -11.24106  -11.24095
 -11.23973  -11.23900  -11.23875  -11.23858  -11.23844  -11.23226
 -11.22501   -1.37812   -1.24651   -1.16925   -1.14295   -1.10953
  -1.03367   -1.01922   -1.01501   -1.00848   -0.94572   -0.93727
  -0.85525   -0.83859   -0.82928   -0.82346   -0.78547   -0.72894
  -0.70784   -0.69302   -0.66771   -0.65598   -0.63960   -0.63318
  -0.62732   -0.61241   -0.60570   -0.60029   -0.59331   -0.58483
  -0.57654   -0.56336   -0.54773   -0.54100   -0.52244   -0.51845
  -0.51645   -0.50676   -0.50121   -0.49229   -0.48309   -0.47309
  -0.46665   -0.41640   -0.40777   -0.34208   -0.33746   -0.32594
  -0.30079    0.12588    0.13248    0.13692    0.14883    0.19406
   0.22831    0.23459    0.24692    0.26017    0.26392

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H1      8.997518E-04   8.927038E-03   1.651197E-02
   2    C1      2.156175E-04   1.193059E-03  -5.081797E-03
   3    C2      1.377866E-03   1.434696E-03   7.770498E-03
   4    C3     -5.157992E-03   1.584632E-02   2.338222E-03
   5    C4     -2.340849E-03   7.110679E-03  -7.813980E-03
   6    C5     -1.147408E-03   6.380521E-03  -1.693814E-03
   7    C6     -2.707703E-03  -3.414009E-03   1.026601E-02
```

```
 8    C7      2.372971E-02  -3.756886E-03   3.379968E-03
 9    H3      3.230621E-03  -7.362990E-03   1.099796E-02
10    H4      3.220901E-03  -1.345732E-02  -8.237696E-04
11    H6     -2.481048E-04  -9.449784E-03  -1.461730E-02
12    H7     -2.019941E-02  -3.787618E-03   1.997602E-03
13    C10     4.604323E-03  -5.148018E-03  -1.123617E-02
14    C8      1.522449E-02  -1.002481E-02   2.748988E-03
15    C17    -2.282109E-02  -3.159582E-03   1.160608E-03
16    N2      9.527139E-03  -1.921381E-02  -2.997208E-02
17    C9      2.336285E-02   1.305733E-02   5.283429E-02
18    C16    -1.926816E-03  -3.772220E-03   8.688964E-03
19    O1     -1.992287E-02   1.724732E-02  -3.903475E-02
20    C11    -1.325901E-03  -4.946514E-03  -7.433820E-03
21    C12     2.158934E-03  -2.953273E-04   1.052682E-03
22    C13    -6.841971E-03   2.158855E-03   1.744087E-03
23    C14    -8.184736E-03   1.412389E-03  -1.044596E-03
24    C15     4.307498E-03  -6.397625E-03  -5.283559E-03
25    H19    -1.380148E-02   2.371939E-03  -4.250498E-03
26    H20     1.020278E-02  -1.010793E-02  -1.027671E-02
27    H21     1.285188E-02  -1.383261E-03   4.225558E-03
28    H22    -8.606424E-03   8.096130E-03   6.687479E-03
29    H23     4.313868E-03   6.735936E-03   1.097202E-02
30    H27     4.774694E-03  -7.749592E-03   1.317482E-03
31    H29     5.586975E-03   5.473708E-03   9.484426E-03
32    H30    -5.564505E-03   2.273357E-02   8.181955E-03
33    H15     4.091202E-03   4.153305E-03  -7.287114E-03
34    H2     -8.387129E-03  -9.390338E-03  -2.799445E-04
35    H5     -1.168720E-02   2.602225E-03  -1.186952E-02
36    H8      7.414975E-03  -3.622704E-03  -5.516214E-03
----------   -------------  -------------  -------------
  total       2.244773E-04   4.946797E-04  -1.154878E-03

 end of program der1b


 start of program geopt   1

 geometry optimization step  1
 reading input hessian of dimension   108
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3000741
  Cos(theta):   0.7984203

  Final level shift:  -5.8398525E-02

 gradient maximum:        4.6520E-02 .  (  4.5000E-04 )
 gradient rms:            1.1108E-02 .  (  3.0000E-04 )
 step size:   0.30007  trust radius:   0.30000
 displacement maximum:    1.1105E-01 .  (  1.8000E-03 )
```

```
  displacement rms:        2.7167E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.7327E-02    geom step:   3.0007E-
01    full step:   3.0007E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.6523E-02     y:     8.9915E-03     z:    -2.5956E-02

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -0.1125544004     1.3490182705    -2.0812065928
  C1       -0.0822700274     1.7742139994    -1.0960895655
  C2        0.0290323561     2.9020261661     1.3957088232
  C3        0.2557395309     0.9718435547    -0.0179704405
  C4       -0.3738000657     3.1170338190    -0.9481893897
  C5       -0.3294276373     3.6736671945     0.3057929409
  C6        0.3499836997     1.5588462521     1.2414057048
  C7        0.6122424529    -0.4980057977    -0.1556845847
  H3       -0.6350433020     3.7104071981    -1.8061834164
  H4       -0.5694629196     4.7118682444     0.4490663105
  H6        0.0619705995     3.3609698431     2.3660311927
  H7        1.7034409118    -0.5385367759    -0.1989842631
  C10       0.1054851835    -1.2098512322    -1.3996296773
  C8        0.2078252075    -1.2521636252     1.1329248539
  C17      -1.3040113438    -1.3954332180     1.3761425972
  N2        0.7568932496     0.7974509187     2.3693619131
  C9        0.8392743886    -0.5812616526     2.3405009354
  C16       1.3562820162     1.4790377411     3.5226830965
  O1        1.3273195924    -1.2228601031     3.2178176845
  C11      -0.7761848500    -2.6390271913    -3.6419126009
  C12       0.9705567267    -2.0335882352    -2.1084272016
  C13      -1.2128116490    -1.1138195693    -1.8367723249
  C14      -1.6518122708    -1.8195067100    -2.9435818449
  C15       0.5393641985    -2.7434115200    -3.2201161282
  H19       1.9950673825    -2.1306678967    -1.7916213106
  H20      -1.9066696388    -0.4885860461    -1.3064888263
  H21      -2.6766917841    -1.7336993858    -3.2588816819
  H22       1.2280204278    -3.3744941707    -3.7559404525
  H23      -1.1161528266    -3.1883795484    -4.5025636783
  H27      -1.8132497488    -0.4352163135     1.3515607326
  H29      -1.7474827154    -2.0330232700     0.6237774500
  H30       0.6389800842    -2.2479882977     1.0994689308
  H15      -1.4778959657    -1.8495380113     2.3443816832
  H2        2.0206296056     2.2677146093     3.1671030759
  H5        1.8975484632     0.7522382677     4.1236662018
  H8        0.5750960993     1.9314319120     4.1373180039

  nuclear repulsion energy.......  1398.698128140 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   1   /
 ------------------------------------------------
```

```
  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.273E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     86     86     89     89     87     87
81
  grid # 2      115     96     95     99     97     97     98
89
  grid # 3      210    183    182    194    182    183    187
176
  grid # 4      208    327    327    339    325    327    329
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     66     92     82     72
96
  grid # 2      118    118    113    106    100     92     79
105
  grid # 3      223    223    208    210    196    173    150
215
  grid # 4      223    223    208    205    340    317    288
394

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       82     73    110     89     88     87     89
89
  grid # 2       92     80    122     97     95     95     95
97
  grid # 3      173    145    258    184    182    182    183
185
  grid # 4      293    274    455    328    326    325    326
327
```

```
  number of gridpoints:
     atom        H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1        72     69     73     73     73     72     71
69
  grid # 2       113    111    118    118    118    109    109
109
  grid # 3       214    209    223    222    224    214    210
215
  grid # 4       213    205    223    224    224    211    206
208

  number of gridpoints:
     atom        H15     H2     H5     H8  total
  grid # 1        71     72     71     71   2864
  grid # 2       109    109    107    111   3731
  grid # 3       219    216    214    216   7183
  grid # 4       219    221    216    223   9939

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
       r  t  s  t  d     total energy   change  change    error

etot   1  N  N  2  U  -783.01451419036           3.2E-04  6.7E-03
etot   2  Y  Y  6  M  -783.02712585440  1.3E-02  1.2E-04  1.9E-03
etot   3  N  Y  2  U  -783.02832733897  1.2E-03  4.2E-05  7.4E-04
etot   4  Y  Y  6  M  -783.02848671427  1.6E-04  1.8E-05  2.4E-04
etot   5  Y  Y  6  M  -783.02851057783  2.4E-05  6.8E-06  1.0E-04
etot   6  Y  Y  6  M  -783.02851766483  7.1E-06  2.8E-06  3.3E-05
etot   7  Y  N  6  M  -783.02851948313  1.8E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1398.69812813984
   (E)  Total one-electron terms..... -3841.80557777224
   (I)  Total two-electron terms.....  1660.07893014927
   (L)  Electronic energy............. -2181.72664762297  (E+I)
   (N)  Total energy.................  -783.02851948313  (A+L)

 SCFE: SCF energy: HF    -783.02851948313 hartrees   iterations:
7
```

```
HOMO energy:    -0.30278
LUMO energy:     0.12996

 Orbital energies:
 -20.52777  -15.59956  -11.34431  -11.28540  -11.25842  -11.25141
 -11.24404  -11.24241  -11.24004  -11.23570  -11.23560  -11.23541
 -11.23380  -11.23370  -11.23340  -11.23278  -11.23251  -11.22661
 -11.21915   -1.40009   -1.26498   -1.16861   -1.15033   -1.10686
  -1.03202   -1.02122   -1.01901   -1.01524   -0.95301   -0.93941
  -0.85628   -0.84624   -0.83308   -0.82885   -0.79003   -0.73952
  -0.71012   -0.69676   -0.67152   -0.65989   -0.64750   -0.63561
  -0.63350   -0.61560   -0.61281   -0.60180   -0.59509   -0.58652
  -0.57718   -0.56623   -0.55292   -0.54857   -0.52641   -0.52087
  -0.51827   -0.51106   -0.50428   -0.49248   -0.48471   -0.47541
  -0.46680   -0.42072   -0.40711   -0.34138   -0.33651   -0.32665
  -0.30278    0.12996    0.13581    0.14032    0.15016    0.21038
   0.23406    0.23945    0.25603    0.26331    0.26800

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H1     -2.843948E-04  -1.768825E-03   3.816059E-04
  2    C1      4.013632E-04  -2.107590E-03  -3.990825E-03
  3    C2      1.880646E-03   2.399328E-03   4.206897E-03
  4    C3      2.260431E-05  -1.542721E-03  -6.428492E-03
  5    C4     -8.246208E-04  -3.075724E-05  -5.869721E-03
  6    C5     -1.408096E-04   4.495031E-03   5.329121E-03
  7    C6     -4.100620E-03  -1.476936E-03   1.073927E-02
  8    C7      1.675477E-03  -1.597375E-03   1.942409E-03
  9    H3      9.079074E-05  -1.735100E-04  -4.749835E-05
 10    H4      2.878944E-06   5.060941E-04   6.681287E-04
 11    H6     -8.561721E-05  -1.196431E-03  -2.860196E-04
 12    H7     -2.072512E-03  -1.106956E-03   5.557557E-04
 13    C10     1.254851E-03   4.882624E-04  -1.063035E-03
 14    C8      1.329381E-03  -9.391682E-04   2.572407E-04
 15    C17     7.257762E-05   2.118546E-03  -9.601074E-04
 16    N2      1.176564E-02  -5.294806E-03   2.330405E-03
```

```
  17    C9     -9.605992E-03   1.031359E-02  -1.519911E-02
  18    C16    -5.552208E-03   2.799024E-03  -8.704006E-04
  19    O1      4.833917E-03  -3.935250E-03   1.132899E-02
  20    C11     8.406961E-04   2.580410E-04   4.894653E-04
  21    C12     1.156232E-03  -1.395091E-03  -1.516834E-03
  22    C13    -2.383016E-03  -4.002380E-04  -2.034229E-04
  23    C14     1.420427E-03  -1.247136E-03  -5.713953E-04
  24    C15    -1.961764E-03  -8.413992E-06  -6.780641E-04
  25    H19     9.185237E-05   6.970024E-04   2.386755E-04
  26    H20     6.566934E-05   1.072920E-03  -6.224180E-04
  27    H21    -2.010110E-04   3.441211E-04  -4.557045E-05
  28    H22    -6.697296E-05   4.906855E-04   7.863280E-04
  29    H23     1.007612E-04   2.247392E-04   1.475222E-04
  30    H27     8.470764E-04  -1.305380E-03   6.115242E-04
  31    H29    -4.006935E-04  -6.083159E-04   2.988882E-04
  32    H30    -2.181455E-04   2.027391E-03   5.235741E-04
  33    H15     3.826738E-04  -1.800988E-04   8.157158E-04
  34    H2     -1.258469E-03  -4.917652E-03   3.649656E-03
  35    H5     -3.387698E-03   5.274773E-03  -6.376292E-03
  36    H8      4.567347E-03  -1.655723E-03  -1.393586E-03
 -----------   -------------  -------------  -------------
    total       2.583143E-04   6.211741E-04  -8.216112E-04

  end of program der1b


  start of program geopt   2

  geometry optimization step  2
  reading input hessian of dimension   108
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3001113
   Cos(theta):   0.3438790

   Final level shift:  -9.0558376E-03

  energy change:          -1.5420E-02 .  (  5.0000E-05 )
  gradient maximum:        1.2466E-02 .  (  4.5000E-04 )
  gradient rms:            2.8676E-03 .  (  3.0000E-04 )
  step size:   0.30007  trust radius:   0.30000
  displacement maximum:    1.5640E-01 .  (  1.8000E-03 )
  displacement rms:        2.7167E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.0421E-03    geom step:   3.0007E-
01    full step:   3.0007E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     2.6876E-03     y:     3.5458E-03     z:    -8.0629E-03
```

new geometry:

atom	x	y	z
		angstroms	
H1	-0.1836293277	1.3519229579	-2.0807243168
C1	-0.1206287408	1.7799884914	-1.0997595757
C2	0.0724565960	2.9124184503	1.4091953925
C3	0.2449834514	0.9763117560	-0.0312145508
C4	-0.3998045224	3.1291402110	-0.9335988731
C5	-0.3142312264	3.6881567674	0.3296428650
C6	0.3776239045	1.5651664822	1.2377585711
C7	0.5992583822	-0.4991027587	-0.1644418778
H3	-0.6832165432	3.7268328662	-1.7801734059
H4	-0.5460070999	4.7253692496	0.4842957080
H6	0.1373634472	3.3631548642	2.3779859680
H7	1.6850756961	-0.5457723000	-0.2075348970
C10	0.0977751432	-1.2180272449	-1.4102646955
C8	0.2078461413	-1.2431026764	1.1326974093
C17	-1.2989569217	-1.3922420662	1.3980762894
N2	0.8385400548	0.8010443436	2.3310507530
C9	0.8404882641	-0.5656353176	2.3318711499
C16	1.3436032579	1.4752974698	3.5298564784
O1	1.2698762047	-1.2028956519	3.2540755479
C11	-0.7690094451	-2.6649111817	-3.6506620540
C12	0.9684797306	-2.0423325494	-2.1109107537
C13	-1.2211959885	-1.1295016146	-1.8573155020
C14	-1.6495480710	-1.8445789613	-2.9634068997
C15	0.5428175506	-2.7617204618	-3.2189637938
H19	1.9909516735	-2.1272437526	-1.7900024676
H20	-1.9164275239	-0.4933786817	-1.3444592426
H21	-2.6702780501	-1.7576435119	-3.2884666289
H22	1.2376876448	-3.3918955944	-3.7428222331
H23	-1.1004328414	-3.2174686627	-4.5104990417
H27	-1.8080847217	-0.4357200124	1.4061211898
H29	-1.7576777852	-2.0170911335	0.6466664807
H30	0.6476887234	-2.2291589587	1.1075661940
H15	-1.4469893645	-1.8654584332	2.3615688531
H2	2.0537110824	2.2425234021	3.2389809718
H5	1.8322222987	0.7343175670	4.1543515305
H8	0.5316980518	1.9343973670	4.1015280406

nuclear repulsion energy..... 1396.934055757 hartrees

```
/  end of geometry optimization iteration   2   /
```

end of program geopt

start of program onee
smallest eigenvalue of S: 3.403E-04
number of canonical orbitals.....   368
end of program onee

```
  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     87     89     88     89     89     87
82
  grid # 2      115     96     95     97     97     97     94
90
  grid # 3      210    184    183    192    182    184    191
175
  grid # 4      208    327    327    340    327    327    328
314

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     66     92     82     72
94
  grid # 2      118    118    110    105    100     90     80
104
  grid # 3      223    223    207    208    194    175    147
214
  grid # 4      224    223    206    207    339    314    286
393

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     72    110     89     88     87     89
89
  grid # 2       90     79    122     97     95     95     95
97
  grid # 3      175    145    259    184    182    183    183
184
  grid # 4      295    276    454    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     71
69
  grid # 2      113    112    118    118    118    109    109
108
```

```
  grid # 3      214    209    223    223    224    215    210
215
  grid # 4      213    205    223    223    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2864
  grid # 2      109    111    107    111   3719
  grid # 3      219    217    212    215   7183
  grid # 4      219    215    212    221   9930

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
       r  t  s  t  d     total energy   change  change    error

etot   1  N  N  2  U  -783.01935918201           2.6E-04  5.9E-03
etot   2  Y  Y  6  M  -783.02884355997  9.5E-03  1.0E-04  1.6E-03
etot   3  N  Y  2  U  -783.02989698669  1.1E-03  2.6E-05  5.0E-04
etot   4  Y  Y  6  M  -783.02996542314  6.8E-05  1.4E-05  2.5E-04
etot   5  Y  Y  6  M  -783.02998857111  2.3E-05  4.7E-06  7.9E-05
etot   6  Y  N  6  M  -783.02999082193  2.3E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1396.93405575700
   (E)  Total one-electron terms..... -3838.25424096586
   (I)  Total two-electron terms.....  1658.29019438693
   (L)  Electronic energy............. -2179.96404657893  (E+I)
   (N)  Total energy.................  -783.02999082193  (A+L)

 SCFE: SCF energy: HF    -783.02999082193 hartrees   iterations:
6


 HOMO energy:    -0.29991
 LUMO energy:     0.12972

  Orbital energies:
  -20.52396  -15.60189  -11.34361  -11.28668  -11.25802  -11.25153
  -11.24498  -11.24397  -11.24017  -11.23733  -11.23574  -11.23537
  -11.23516  -11.23383  -11.23342  -11.23318  -11.23305  -11.22839
```

```
 -11.21890   -1.39515   -1.26855   -1.16797   -1.14815   -1.10719
  -1.03264   -1.02097   -1.01791   -1.01544   -0.95661   -0.94006
  -0.85723   -0.84868   -0.83206   -0.82960   -0.78977   -0.74186
  -0.71094   -0.69797   -0.67012   -0.66105   -0.64769   -0.63574
  -0.63363   -0.61724   -0.61040   -0.60126   -0.59924   -0.58698
  -0.57754   -0.56649   -0.55205   -0.54564   -0.52533   -0.52101
  -0.51845   -0.51172   -0.50437   -0.49294   -0.48321   -0.47599
  -0.46687   -0.42037   -0.40796   -0.34120   -0.33698   -0.32766
  -0.29991    0.12972    0.13421    0.14014    0.14901    0.20871
   0.23397    0.24087    0.25635    0.26356    0.26841

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
   1    H1     -3.342399E-04  -1.014829E-03  -7.603331E-04
   2    C1     -3.554893E-05   1.550356E-03   2.000718E-03
   3    C2      1.342205E-03  -2.276416E-03  -1.346762E-03
   4    C3      9.942566E-04   8.629607E-04   1.777452E-03
   5    C4      3.221399E-04   5.615743E-04   3.277667E-03
   6    C5     -4.590701E-04  -2.763821E-03  -4.068788E-03
   7    C6     -2.934787E-03   1.491936E-05  -2.581718E-03
   8    C7     -1.269782E-03   7.307403E-04   2.603704E-04
   9    H3     -1.382797E-04   4.871283E-04  -4.343152E-04
  10    H4     -8.671782E-05   1.362296E-03  -9.159273E-05
  11    H6      2.243184E-04   4.664835E-04   1.131961E-03
  12    H7      1.469781E-03   1.023994E-04   1.312987E-04
  13    C10    -2.164766E-03   1.055046E-03   1.007445E-04
  14    C8      4.195795E-04   1.427879E-03  -7.921187E-04
  15    C17     1.687143E-03  -2.257025E-04   9.402869E-04
  16    N2      3.733391E-03   4.098949E-03   7.163126E-03
  17    C9     -2.385924E-03  -2.637518E-03   4.484965E-06
  18    C16    -1.635327E-03  -1.574502E-03   1.394982E-03
  19    O1     -4.677502E-04  -1.514818E-03  -8.131952E-04
  20    C11     1.805062E-03   7.263183E-05   1.023001E-03
  21    C12    -7.642356E-04  -8.609758E-04  -1.401140E-03
  22    C13     1.158993E-03  -7.530626E-04  -5.490111E-04
  23    C14     6.666767E-04   1.023733E-03   1.133059E-03
  24    C15    -7.713480E-04   7.480252E-04   3.591316E-04
```

```
  25    H19     1.328721E-03  -1.045286E-04   3.009214E-04
  26    H20    -8.443342E-04   8.660801E-04   5.384705E-04
  27    H21    -9.734845E-04   1.348959E-04  -2.145368E-04
  28    H22     8.408569E-04  -6.496193E-04  -5.159386E-04
  29    H23    -2.626022E-04  -5.628363E-04  -7.194628E-04
  30    H27    -2.776281E-04   1.029185E-03  -4.749714E-05
  31    H29    -7.231794E-04  -1.049745E-03  -1.120228E-03
  32    H30     2.920974E-04  -2.241580E-03  -2.674646E-04
  33    H15    -6.786133E-05  -8.287318E-05   6.334442E-04
  34    H2     -9.501029E-04  -6.509092E-04   1.396432E-03
  35    H5     -2.900340E-03   5.028536E-03  -4.808414E-03
  36    H8      4.273847E-03  -2.722879E-03  -3.769961E-03
 -----------   -------------  -------------  -------------
    total       1.117595E-04  -6.279553E-05  -7.349253E-04

  end of program der1b


  start of program geopt   3

  geometry optimization step  3
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -1.4713E-03 .  (  5.0000E-05 )
  gradient maximum:        7.5031E-03 .  (  4.5000E-04 )
  gradient rms:            1.6310E-03 .  (  3.0000E-04 )
  step size:   0.23051  trust radius:   0.30000
  displacement maximum:    1.5798E-01 .  (  1.8000E-03 )
  displacement rms:        2.0870E-02 .  (  1.2000E-03 )
  predicted energy change:    -8.1419E-04    geom step:   2.3051E-
01    full step:   2.3051E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.2100E-02     y:    -1.8397E-03     z:     1.2163E-02

  new geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -0.2459569282      1.3373998127     -2.0654368470
  C1       -0.1576603769      1.7760798243     -1.0886164867
  C2        0.0930773543      2.9162127566      1.4136375488
  C3        0.2218854675      0.9746865882     -0.0226047786
  C4       -0.4206418575      3.1295424371     -0.9230052816
  C5       -0.3038432997      3.6935491719      0.3365743181
  C6        0.3712262324      1.5643156865      1.2443804944
  C7        0.5736033689     -0.5016475288     -0.1489946594
  H3       -0.7131901046      3.7273364480     -1.7677832653
```

```
 H4       -0.5176610514      4.7356371035      0.4914181882
 H6        0.1815298805      3.3658635066      2.3812966787
 H7        1.6608838932     -0.5540158107     -0.1673371050
 C10       0.1004323297     -1.2182582990     -1.4085871897
 C8        0.1606163308     -1.2402501129      1.1425560300
 C17      -1.3463753081     -1.3705266738      1.4040705491
 N2        0.8249892683      0.8038003707      2.3434555912
 C9        0.7903834594     -0.5686604200      2.3441459612
 C16       1.4476987723      1.4632014169      3.4572474847
 O1        1.1744507790     -1.2161939329      3.2883205113
 C11      -0.6952726953     -2.6654347310     -3.6702314646
 C12       1.0006558772     -2.0241090874     -2.1007402109
 C13      -1.2118547816     -1.1464657357     -1.8775304313
 C14      -1.6034863976     -1.8614435296     -2.9953619444
 C15       0.6090385137     -2.7438072462     -3.2184927835
 H19       2.0203575559     -2.0880813071     -1.7610949610
 H20      -1.9255705755     -0.5172162409     -1.3789160329
 H21      -2.6191191736     -1.7871445324     -3.3430243705
 H22       1.3260066680     -3.3584191707     -3.7320600460
 H23      -1.0028167557     -3.2181019287     -4.5402522864
 H27      -1.8427797435     -0.4082123451      1.4016509204
 H29      -1.8121279735     -2.0003114425      0.6599411823
 H30       0.5882473945     -2.2330182017      1.1222453379
 H15      -1.4999068173     -1.8287604125      2.3730252419
 H2        2.0883760050      2.2563192096      3.1296676109
 H5        2.0248930090      0.7288058451      3.9663158922
 H8        0.7149526944      1.8735365570      4.1264887358

 nuclear repulsion energy.......  1397.214819407 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   3   /
 ------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.417E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H1     C1     C2     C3     C4     C5     C6
C7
```

grid # 1	71	88	88	88	89	89	85
82							
grid # 2	115	96	95	97	97	97	93
90							
grid # 3	210	184	183	192	183	184	189
175							
grid # 4	209	327	326	340	327	327	326
314							

number of gridpoints:

atom	H3	H4	H6	H7	C10	C8	C17
N2							
grid # 1	73	73	70	68	92	82	74
96							
grid # 2	118	118	113	107	100	90	80
106							
grid # 3	223	223	208	209	197	175	151
211							
grid # 4	224	223	207	206	341	314	286
391							

number of gridpoints:

atom	C9	C16	O1	C11	C12	C13	C14
C15							
grid # 1	82	69	111	89	88	87	89
89							
grid # 2	90	76	122	97	95	95	95
97							
grid # 3	175	139	259	184	183	183	183
184							
grid # 4	296	270	453	328	326	325	326
328							

number of gridpoints:

atom	H19	H20	H21	H22	H23	H27	H29
H30							
grid # 1	72	69	73	73	73	72	71
69							
grid # 2	112	112	118	118	118	109	108
108							
grid # 3	214	209	223	223	224	215	210
215							
grid # 4	213	206	223	223	224	210	207
208							

number of gridpoints:

atom	H15	H2	H5	H8	total
grid # 1	71	71	70	71	2867
grid # 2	110	111	107	111	3721
grid # 3	219	216	212	216	7183
grid # 4	217	213	208	213	9905

```
  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  2  U  -783.01774798020             2.4E-04  6.3E-03
etot  2  Y  Y  6  M  -783.02795381847  1.0E-02     1.1E-04  2.0E-03
etot  3  N  Y  2  U  -783.02906619843  1.1E-03     2.7E-05  5.5E-04
etot  4  Y  Y  6  M  -783.02911839587  5.2E-05     1.2E-05  1.6E-04
etot  5  Y  Y  6  M  -783.02913119772  1.3E-05     3.9E-06  9.5E-05
etot  6  Y  N  6  M  -783.02913170307  5.1E-07     0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1397.21481940656
   (E)  Total one-electron terms..... -3838.74482649495
   (I)  Total two-electron terms.....  1658.50087538533
   (L)  Electronic energy............. -2180.24395110962  (E+I)
   (N)  Total energy.................  -783.02913170307  (A+L)

 SCFE: SCF energy: HF    -783.02913170307 hartrees   iterations:
6


 HOMO energy:    -0.30091
 LUMO energy:     0.12932

  Orbital energies:
  -20.52465  -15.60127  -11.34517  -11.28601  -11.25202  -11.24901
  -11.24587  -11.24468  -11.24094  -11.23826  -11.23643  -11.23601
  -11.23577  -11.23446  -11.23408  -11.23372  -11.23367  -11.22961
  -11.21873   -1.39152   -1.27182   -1.16864   -1.14890   -1.10837
   -1.03348   -1.02095   -1.01967   -1.01628   -0.96075   -0.94061
   -0.85782   -0.84875   -0.83277   -0.82964   -0.79034   -0.74252
   -0.71262   -0.69888   -0.66988   -0.66285   -0.64925   -0.63697
   -0.63429   -0.61803   -0.61098   -0.60322   -0.60106   -0.58784
   -0.57860   -0.56702   -0.55216   -0.54948   -0.52369   -0.52081
   -0.51929   -0.51135   -0.50435   -0.49314   -0.48322   -0.47602
   -0.46762   -0.41888   -0.40883   -0.34156   -0.33708   -0.32845
   -0.30091    0.12932    0.13397    0.13944    0.14833    0.20533
    0.23283    0.24136    0.25556    0.26560    0.26836

  end of program scf
```

```
 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	2.627423E-04	6.305812E-04	5.646277E-04
2	C1	1.118506E-05	3.926511E-04	1.481017E-03
3	C2	-4.614730E-04	-1.360367E-03	-2.751770E-03
4	C3	7.862357E-04	6.561085E-04	2.558749E-03
5	C4	3.702546E-04	5.981397E-04	3.487374E-03
6	C5	2.009519E-04	-2.962023E-03	-3.491589E-03
7	C6	-2.625994E-03	1.514516E-03	-4.109026E-03
8	C7	-1.163766E-03	5.306357E-04	-1.363995E-03
9	H3	-6.107692E-05	3.009575E-05	2.795856E-04
10	H4	1.128423E-06	6.032104E-04	-3.521819E-04
11	H6	-2.404901E-04	8.945658E-04	1.255257E-03
12	H7	7.830107E-04	8.331785E-04	-2.344522E-04
13	C10	6.452154E-04	-6.333813E-04	3.728082E-04
14	C8	4.548201E-04	1.164040E-03	-9.650199E-04
15	C17	4.735298E-04	-7.346267E-04	1.245593E-04
16	N2	5.432662E-04	-9.227437E-03	-1.710225E-02
17	C9	-9.229553E-04	-4.058971E-03	1.398708E-02
18	C16	-6.972383E-04	3.880341E-04	5.499905E-03
19	O1	-1.780236E-03	7.098019E-03	-1.119158E-02
20	C11	-1.568856E-03	4.805379E-04	-5.217755E-05
21	C12	-1.272879E-03	2.088187E-03	2.326503E-03
22	C13	2.230752E-03	2.352494E-04	2.955855E-04
23	C14	-8.304591E-05	-6.579453E-04	-1.323174E-03
24	C15	3.931765E-04	1.577437E-04	1.823725E-04
25	H19	5.157714E-05	-2.913309E-04	-8.786961E-05
26	H20	-3.140829E-04	-2.290893E-04	4.600263E-04
27	H21	-6.117807E-05	-1.827979E-04	-4.161668E-05
28	H22	2.743296E-04	-4.847503E-04	-5.998476E-04
29	H23	-1.768870E-04	-1.024634E-04	-1.684879E-05
30	H27	-7.941422E-04	1.417362E-03	-3.267716E-04
31	H29	-5.084514E-04	-5.879024E-04	-1.075489E-03
32	H30	2.942670E-04	-1.347167E-03	5.685689E-05
33	H15	-2.382979E-04	-4.975423E-04	9.190023E-04
34	H2	5.109080E-03	5.721265E-03	-5.423007E-03
35	H5	5.252299E-03	-4.505101E-03	8.683373E-03
36	H8	-4.938977E-03	2.539189E-03	7.181697E-03

```
 -----------   -------------  -------------  -------------
    total       2.277937E-04   1.104140E-04  -7.922917E-04

  end of program der1b


  start of program geopt   4

  geometry optimization step  4
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  ** restarting optimization from step    3 **


  energy change:           8.5912E-04 .  (  5.0000E-05 )
  gradient maximum:        7.5031E-03 .  (  4.5000E-04 )
  gradient rms:            1.6310E-03 .  (  3.0000E-04 )
  step size:   0.17216  trust radius:   0.30000
  displacement maximum:    8.9355E-02 .  (  1.8000E-03 )
  displacement rms:        1.5586E-02 .  (  1.2000E-03 )
  predicted energy change:    -6.2212E-04    geom step:   1.7216E-
01    full step:   1.7216E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.1102E-16     y:    -2.4980E-16     z:    -2.2204E-16

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -0.2553649141     1.3372222433    -2.0639036299
  C1       -0.1634617567     1.7743205951    -1.0859752402
  C2        0.1040073922     2.9130754171     1.4007181924
  C3        0.2287776766     0.9747216627    -0.0246003701
  C4       -0.4328399227     3.1240573798    -0.9247832476
  C5       -0.3077771016     3.6860326734     0.3263027550
  C6        0.3879527889     1.5638856149     1.2341652320
  C7        0.5834790355    -0.4976302041    -0.1573698983
  H3       -0.7353751875     3.7175117102    -1.7693550008
  H4       -0.5227298621     4.7287329282     0.4809300874
  H6        0.2019049747     3.3723705574     2.3664583620
  H7        1.6725242770    -0.5426241025    -0.1909732639
  C10       0.0936422042    -1.2153693552    -1.4073270987
  C8        0.1838649810    -1.2424013184     1.1361319200
  C17      -1.3235968780    -1.3788727628     1.4051209590
  N2        0.8847145608     0.7999427402     2.3167307864
  C9        0.8187664664    -0.5751604381     2.3395223477
  C16       1.3744985784     1.4658025737     3.5140521545
  O1        1.2225939044    -1.2253812821     3.2634648836
  C11      -0.7385426050    -2.6628990657    -3.6536551581
```

```
  C12       0.9798828225     -2.0271824754     -2.1062658564
  C13      -1.2222518806     -1.1383956356     -1.8605009060
  C14      -1.6340207402     -1.8528618803     -2.9707361376
  C15       0.5718499227     -2.7471692180     -3.2176692258
  H19       2.0033759919     -2.0996586765     -1.7782345208
  H20      -1.9280510027     -0.5098897923     -1.3497012977
  H21      -2.6545372084     -1.7775907272     -3.3030911777
  H22       1.2779339660     -3.3688575097     -3.7398455445
  H23      -1.0604366769     -3.2188373218     -4.5169112486
  H27      -1.8244582485     -0.4159884213      1.4086644039
  H29      -1.7902746586     -2.0032003878      0.6557662839
  H30       0.6115222371     -2.2378721009      1.1088521860
  H15      -1.4746684235     -1.8438661068      2.3715021479
  H2        2.0877143373      2.2365658426      3.2382978931
  H5        1.8463455099      0.7332576469      4.1302834590
  H8        0.5670645365      1.9153701228      4.0720034372

  nuclear repulsion energy.......  1397.566331693 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   4   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.327E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     87     89     88     89     87     85
81
  grid # 2      115     96     95     98     97     97     95
90
  grid # 3      210    184    183    192    182    183    193
176
  grid # 4      208    327    326    336    327    327    329
311

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
```

```
  grid # 1       73     73     70     66     92     81     73
95
  grid # 2      118    118    111    107    100     90     80
104
  grid # 3      223    223    207    207    197    175    148
216
  grid # 4      224    223    207    206    341    315    288
391

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     69    110     89     88     87     89
89
  grid # 2       91     78    122     97     95     95     95
97
  grid # 3      175    144    259    184    183    183    183
184
  grid # 4      295    274    454    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     71
69
  grid # 2      113    112    118    118    118    109    109
109
  grid # 3      214    209    223    223    224    215    210
215
  grid # 4      213    205    223    224    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2857
  grid # 2      110    111    106    109   3723
  grid # 3      219    217    214    216   7193
  grid # 4      217    217    209    214   9915

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
```

```
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  2  U  -783.02007187364           2.4E-04  8.3E-03
etot   2  Y  Y  6  M  -783.02927950792  9.2E-03  1.0E-04  2.3E-03
etot   3  N  Y  2  U  -783.03020522889  9.3E-04  2.8E-05  6.4E-04
etot   4  Y  Y  6  M  -783.03027940899  7.4E-05  1.2E-05  2.4E-04
etot   5  Y  Y  6  M  -783.03028503421  5.6E-06  3.6E-06  6.0E-05
etot   6  Y  N  6  M  -783.03028606742  1.0E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1397.56633169276
   (E)  Total one-electron terms..... -3839.49004995798
   (I)  Total two-electron terms.....  1658.89343219781
   (L)  Electronic energy............. -2180.59661776018  (E+I)
   (N)  Total energy.................  -783.03028606742  (A+L)

 SCFE: SCF energy: HF    -783.03028606742 hartrees   iterations:
6


 HOMO energy:    -0.30151
 LUMO energy:     0.13004

  Orbital energies:
  -20.52575  -15.60168  -11.34527  -11.28578  -11.25374  -11.25134
  -11.24485  -11.24311  -11.24072  -11.23682  -11.23589  -11.23533
  -11.23467  -11.23393  -11.23344  -11.23321  -11.23315  -11.22772
  -11.21944   -1.39556   -1.26862   -1.16869   -1.14964   -1.10760
   -1.03274   -1.02124   -1.01978   -1.01557   -0.95796   -0.93998
   -0.85744   -0.84726   -0.83281   -0.82920   -0.79009   -0.74164
   -0.71168   -0.69813   -0.67055   -0.66154   -0.64823   -0.63530
   -0.63411   -0.61700   -0.61161   -0.60171   -0.60086   -0.58738
   -0.57727   -0.56668   -0.55279   -0.54683   -0.52597   -0.52176
   -0.51768   -0.51233   -0.50448   -0.49273   -0.48307   -0.47689
   -0.46662   -0.42061   -0.40878   -0.34108   -0.33690   -0.32782
   -0.30151    0.13004    0.13527    0.14014    0.14944    0.20701
    0.23354    0.24134    0.25619    0.26452    0.26825

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b
```

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	1.646466E-04	1.880849E-04	1.194528E-03
2	C1	-1.143771E-05	-2.716188E-03	-2.233249E-03
3	C2	7.541546E-05	1.416283E-03	2.505989E-03
4	C3	-4.253961E-04	-4.308706E-04	-2.827206E-03
5	C4	-4.375653E-04	8.236331E-05	-1.517397E-03
6	C5	1.826236E-04	1.468845E-03	2.225074E-03
7	C6	1.890309E-03	2.713480E-04	2.595240E-03
8	C7	2.602789E-04	-4.812970E-04	6.468153E-06
9	H3	5.713597E-05	-9.141122E-05	3.303538E-04
10	H4	7.054680E-05	6.935440E-05	6.101354E-05
11	H6	-6.158785E-05	-3.065612E-04	-1.217761E-03
12	H7	-5.129256E-04	1.551967E-04	2.122968E-04
13	C10	6.175495E-04	1.191041E-04	2.124329E-04
14	C8	-5.224880E-04	-4.036044E-04	1.057044E-04
15	C17	2.647212E-04	8.432808E-04	-1.035454E-03
16	N2	-2.998698E-03	-5.940236E-03	1.516803E-03
17	C9	2.501823E-03	2.303579E-03	-3.416043E-03
18	C16	1.289114E-03	5.198916E-03	-6.440152E-03
19	O1	-1.440233E-03	2.127304E-03	8.438183E-04
20	C11	-5.806567E-04	-3.024552E-04	-6.988772E-04
21	C12	8.317287E-04	6.708537E-04	1.155040E-03
22	C13	1.898071E-04	6.083157E-04	8.280867E-04
23	C14	1.022979E-04	-1.030023E-03	-1.085521E-03
24	C15	-5.602844E-04	-4.244240E-04	-7.314447E-04
25	H19	-2.818396E-04	5.122420E-05	-7.639044E-05
26	H20	-1.349307E-04	1.139769E-04	1.266286E-04
27	H21	-1.031447E-04	3.878404E-05	-8.689889E-05
28	H22	-4.282440E-05	3.212363E-05	-3.567128E-05
29	H23	2.665011E-05	1.359576E-04	9.593062E-05
30	H27	8.621960E-05	-9.910492E-06	-7.450652E-05
31	H29	-3.025603E-04	-4.870089E-04	-2.476128E-04
32	H30	-6.554063E-05	5.796551E-04	-3.542383E-05
33	H15	-3.036731E-05	-4.704390E-04	7.311849E-04
34	H2	-8.466337E-04	-1.158103E-03	1.054078E-03
35	H5	3.975139E-03	-4.172060E-03	3.253721E-03
36	H8	-3.246331E-03	2.092198E-03	1.982446E-03
total		-1.943880E-05	1.421568E-04	-7.227703E-04

end of program der1b

start of program geopt 5

geometry optimization step 5
reading input hessian of dimension 108
in five columns format
reading input hessian of dimension 108

```
 in five columns format
 reading input hessian of dimension   108
 in five columns format


 energy change:          -2.9525E-04 .  (  5.0000E-05 )
 gradient maximum:        6.5112E-03 .  (  4.5000E-04 )
 gradient rms:            1.3323E-03 .  (  3.0000E-04 )
 step size:   0.10676  trust radius:   0.30000
 displacement maximum:    4.7006E-02 .  (  1.8000E-03 )
 displacement rms:        9.6652E-03 .  (  1.2000E-03 )
 predicted energy change:    -3.1709E-04    geom step:   1.0676E-
01    full step:   1.0676E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:    -3.5337E-03     y:     2.9124E-03     z:     2.1934E-03

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -0.2344385411     1.3364228531    -2.0667070982
 C1       -0.1506901513     1.7741528144    -1.0904591912
 C2        0.0955808939     2.9156235693     1.4078351314
 C3        0.2323643835     0.9758613033    -0.0253863064
 C4       -0.4181426541     3.1253566840    -0.9264949330
 C5       -0.3017754596     3.6891436387     0.3286321546
 C6        0.3798253710     1.5651914599     1.2396659215
 C7        0.5896607348    -0.4962320424    -0.1602410297
 H3       -0.7108620707     3.7223672554    -1.7715551535
 H4       -0.5144793653     4.7335487966     0.4797902349
 H6        0.1826731673     3.3746323306     2.3733599051
 H7        1.6786088441    -0.5367428888    -0.1964787350
 C10       0.0972623924    -1.2125831964    -1.4084184665
 C8        0.1938500468    -1.2454542803     1.1305180322
 C17      -1.3126544312    -1.3967971446     1.3890162854
 N2        0.8514294863     0.7972393659     2.3303292176
 C9        0.8189689222    -0.5711590604     2.3353520859
 C16       1.3677897324     1.4697464553     3.5150302751
 O1        1.2303401913    -1.2107769044     3.2628019889
 C11      -0.7487994201    -2.6694740655    -3.6501763233
 C12       0.9774683268    -2.0319907690    -2.1057483750
 C13      -1.2185751344    -1.1313055703    -1.8601168777
 C14      -1.6372039610    -1.8512176390    -2.9679801387
 C15       0.5619182715    -2.7565377345    -3.2152392822
 H19       2.0013675137    -2.1092659092    -1.7790936517
 H20      -1.9218381946    -0.4974916153    -1.3496088765
 H21      -2.6593870529    -1.7717986876    -3.2970586587
 H22       1.2648630101    -3.3848574016    -3.7356945104
 H23      -1.0756366493    -3.2283082760    -4.5096926231
 H27      -1.8236843591    -0.4397355171     1.3843325766
 H29      -1.7665598344    -2.0305719249     0.6392268879
```

```
  H30       0.6325418295     -2.2362990528      1.1023133627
  H15      -1.4677484430     -1.8605599611      2.3568907829
  H2        2.0692522862      2.2421623047      3.2296189653
  H5        1.8687512123      0.7359276318      4.1223141056
  H8        0.5693062719      1.9174617110      4.0954051281

  nuclear repulsion energy.......  1397.567973708 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   5   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.366E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
  grid # 3      210    184    182    192    182    183    194
175
  grid # 4      209    327    327    340    327    327    328
313

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     82     73
96
  grid # 2      118    118    111    107    100     90     80
106
  grid # 3      223    223    207    207    197    174    147
211
  grid # 4      224    223    207    204    341    313    288
392

  number of gridpoints:
```

```
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     69    111     89     88     87     89
89
  grid # 2       90     78    122     97     95     95     95
97
  grid # 3      175    147    259    184    182    182    183
184
  grid # 4      292    274    454    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     71
69
  grid # 2      113    112    118    118    118    109    108
109
  grid # 3      214    209    223    223    224    215    210
214
  grid # 4      213    205    223    224    224    212    207
207

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2863
  grid # 2      109    111    107    111   3722
  grid # 3      219    217    212    215   7182
  grid # 4      218    213    209    216   9914

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS    maximum
       t  p  i  c  r                          energy  density   DIIS
       e  d  i  u  i                          change  change    error
       r  t  s  t  d     total energy

etot   1  N  N  2  U  -783.02910080271                  9.9E-05  2.1E-03
etot   2  Y  Y  6  M  -783.03026808027  1.2E-03  3.6E-05  5.0E-04
etot   3  Y  Y  6  M  -783.03040309899  1.4E-04  1.0E-05  1.3E-04
etot   4  Y  Y  6  M  -783.03040750325  4.4E-06  4.8E-06  7.0E-05
etot   5  Y  N  6  M  -783.03041185602  4.4E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
```

```
   (A)  Nuclear repulsion.....  1397.56797370847
   (E)  Total one-electron terms..... -3839.50158436416
   (I)  Total two-electron terms.....  1658.90319879967
   (L)  Electronic energy..... -2180.59838556449  (E+I)
   (N)  Total energy.................  -783.03041185602  (A+L)

 SCFE: SCF energy: HF    -783.03041185602 hartrees   iterations:
5


 HOMO energy:    -0.30083
 LUMO energy:     0.12971

  Orbital energies:
 -20.52356  -15.60168  -11.34382  -11.28653  -11.25478  -11.25148
 -11.24502  -11.24382  -11.24089  -11.23732  -11.23637  -11.23591
 -11.23491  -11.23439  -11.23391  -11.23363  -11.23346  -11.22826
 -11.21936   -1.39566   -1.26866   -1.16856   -1.14885   -1.10779
  -1.03292   -1.02077   -1.01870   -1.01556   -0.95830   -0.94000
  -0.85719   -0.84802   -0.83250   -0.82937   -0.78967   -0.74169
  -0.71162   -0.69798   -0.67023   -0.66152   -0.64802   -0.63555
  -0.63382   -0.61748   -0.61115   -0.60191   -0.60048   -0.58656
  -0.57768   -0.56651   -0.55208   -0.54617   -0.52530   -0.52140
  -0.51813   -0.51198   -0.50430   -0.49292   -0.48299   -0.47650
  -0.46691   -0.41997   -0.40827   -0.34116   -0.33670   -0.32815
  -0.30083    0.12971    0.13473    0.13974    0.14909    0.20815
   0.23336    0.24099    0.25566    0.26410    0.26811

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x             y             z
 ----  -----   -------------  -------------  -------------
   1    H1     -7.677519E-05   9.231691E-05  -2.085869E-04
   2    C1      2.638254E-04   1.373339E-04   8.801134E-04
   3    C2      3.340346E-04  -4.116849E-04  -1.380336E-04
   4    C3     -1.380576E-04   4.756051E-04   6.968111E-04
   5    C4      5.583649E-05   8.550326E-04   5.674120E-04
   6    C5     -3.172298E-04   1.401291E-04  -9.692243E-04
   7    C6     -1.857771E-04  -6.773380E-04  -4.955440E-05
```

8	C7	6.746545E-04	4.564955E-04	3.065577E-04
9	H3	-1.426525E-04	2.151106E-05	4.214973E-05
10	H4	4.895112E-05	-4.737249E-04	-1.290728E-04
11	H6	8.463041E-05	-3.160262E-04	-2.309591E-04
12	H7	-3.220387E-04	-1.415180E-04	1.012424E-04
13	C10	3.327392E-04	-4.352003E-04	-7.131503E-04
14	C8	5.427940E-04	-4.594948E-04	1.692938E-04
15	C17	-3.938421E-04	-2.278407E-04	2.629914E-04
16	N2	1.450680E-04	3.401701E-03	-1.649495E-03
17	C9	2.732981E-04	-5.776904E-04	8.615798E-05
18	C16	5.898423E-04	-1.257988E-03	3.619358E-04
19	O1	-3.287448E-04	-2.485561E-03	9.162736E-04
20	C11	-7.723931E-05	3.497281E-04	3.113015E-04
21	C12	1.382483E-04	-8.549751E-04	-1.082815E-03
22	C13	-1.459641E-03	-4.229424E-04	-1.063213E-03
23	C14	-2.085096E-04	6.828661E-04	8.048751E-04
24	C15	1.065549E-03	2.696887E-04	8.198818E-04
25	H19	-4.769495E-04	1.486419E-05	-2.783714E-04
26	H20	4.562577E-04	-5.008561E-04	-4.952691E-04
27	H21	4.822561E-04	-4.858213E-06	1.097425E-04
28	H22	-4.113609E-04	4.757333E-04	3.450845E-04
29	H23	8.216108E-05	1.505863E-04	1.296339E-04
30	H27	-5.314500E-05	1.790009E-04	-1.862372E-05
31	H29	-2.122706E-04	-1.563683E-04	-1.181797E-04
32	H30	-1.746330E-04	6.431940E-04	2.759460E-04
33	H15	2.630713E-04	5.479680E-05	4.123383E-05
34	H2	4.232723E-04	7.208649E-04	-1.115212E-03
35	H5	-2.022641E-04	3.705423E-04	-1.116619E-04
36	H8	-9.564148E-04	9.562734E-05	4.305030E-04
total		1.189441E-04	1.835517E-04	-7.122818E-04

 end of program der1b

 start of program geopt   6

 geometry optimization step 6
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format

 energy change: -1.2579E-04 . (5.0000E-05)
 gradient maximum: 3.9949E-03 . (4.5000E-04)
 gradient rms: 7.9005E-04 . (3.0000E-04)
 step size: 0.10684 trust radius: 0.30000
 displacement maximum: 5.2270E-02 . (1.8000E-03)
 displacement rms: 9.6727E-03 . (1.2000E-03)
 predicted energy change: -1.5780E-04   geom step: 1.0684E-
01   full step: 1.0684E-01

```
 molecular structure not yet converged...

 center of mass moved by:
    x:    -6.8973E-03     y:    -1.8351E-03     z:     3.4367E-03

 new geometry:
                                angstroms
 atom            x                 y                 z
 H1       -0.2741512903      1.3380230570     -2.0609177057
 C1       -0.1725178922      1.7735932523     -1.0852572003
 C2        0.1252525523      2.9193573079      1.4041091320
 C3        0.2278596169      0.9764452612     -0.0261866593
 C4       -0.4354563879      3.1260628221     -0.9191494867
 C5       -0.2925082833      3.6921803109      0.3316265415
 C6        0.3989044503      1.5676612824      1.2342033646
 C7        0.5803056497     -0.4971966090     -0.1559710956
 H3       -0.7460372804      3.7206491555     -1.7598040024
 H4       -0.5012009509      4.7355263666      0.4849860661
 H6        0.2335055585      3.3790617275      2.3660491144
 H7        1.6684534895     -0.5421636806     -0.1804297266
 C10       0.0999269605     -1.2159174577     -1.4097148021
 C8        0.1724198069     -1.2402403969      1.1356872967
 C17      -1.3366137596     -1.3842553449      1.3901218274
 N2        0.8750790352      0.7990704072      2.3203115983
 C9        0.7945423570     -0.5726669086      2.3463360528
 C16       1.4100438272      1.4692013331      3.4967352591
 O1        1.1497004023     -1.2224589171      3.2955415282
 C11      -0.7204227544     -2.6704162059     -3.6603281268
 C12       0.9936852451     -2.0184661813     -2.1103964568
 C13      -1.2169305588     -1.1513823228     -1.8638384988
 C14      -1.6228785664     -1.8696838731     -2.9752917407
 C15       0.5911763521     -2.7413941791     -3.2236887911
 H19       2.0167321907     -2.0821224705     -1.7835509958
 H20      -1.9290836252     -0.5325161328     -1.3521740984
 H21      -2.6436735205     -1.8040759109     -3.3067510726
 H22       1.3022417960     -3.3545098117     -3.7472238791
 H23      -1.0370275963     -3.2275355231     -4.5239745698
 H27      -1.8419527167     -0.4243513628      1.3890130596
 H29      -1.7924833813     -2.0123255821      0.6386016041
 H30       0.6061793022     -2.2314107719      1.1131972238
 H15      -1.4934632539     -1.8506460728      2.3552214678
 H2        2.0996127162      2.2456458246      3.1985927063
 H5        1.9269778785      0.7336512853      4.0914252835
 H8        0.6165446113      1.9102440959      4.0937021100

 nuclear repulsion energy.......  1396.727595837 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   6   /
------------------------------------------------

 end of program geopt
```

```
  start of program onee
  smallest eigenvalue of S:    3.367E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     87     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
  grid # 3      210    184    182    192    182    183    192
176
  grid # 4      208    327    327    340    327    327    328
311

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     81     73
94
  grid # 2      118    118    111    106    100     90     80
104
  grid # 3      223    223    207    207    197    175    150
213
  grid # 4      224    223    207    204    341    315    287
391

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     69    110     89     88     87     89
89
  grid # 2       90     79    122     97     95     95     95
97
  grid # 3      176    140    260    184    183    182    183
184
  grid # 4      294    272    455    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
```

```
  grid # 1       72     69     73     73     73     72     70
69
  grid # 2      112    112    118    118    118    109    108
108
  grid # 3      214    209    223    223    224    215    210
215
  grid # 4      213    205    223    224    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2857
  grid # 2      109    111    108    111   3719
  grid # 3      219    216    212    216   7184
  grid # 4      217    213    209    217   9913

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                        energy  density   DIIS
      r  t  s  t  d     total energy       change  change    error

etot  1  N  N  2  U  -783.02656911709                1.5E-04  3.4E-03
etot  2  Y  Y  6  M  -783.03004227068  3.5E-03  6.3E-05  1.0E-03
etot  3  Y  Y  6  M  -783.03046734550  4.3E-04  1.5E-05  2.4E-04
etot  4  N  Y  2  U  -783.03048851925  2.1E-05  7.1E-06  1.3E-04
etot  5  Y  Y  6  M  -783.03049339769  4.9E-06  4.0E-06  5.7E-05
etot  6  Y  N  6  M  -783.03049388296  4.9E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1396.72759583692
   (E)  Total one-electron terms..... -3837.82092731570
   (I)  Total two-electron terms.....  1658.06283759581
   (L)  Electronic energy............. -2179.75808971988  (E+I)
   (N)  Total energy.................  -783.03049388296  (A+L)

 SCFE: SCF energy: HF    -783.03049388296 hartrees   iterations:
6


 HOMO energy:    -0.30100
 LUMO energy:     0.12978
```

Orbital energies:

-20.52505	-15.60225	-11.34540	-11.28608	-11.25556	-11.25135
-11.24520	-11.24363	-11.24076	-11.23722	-11.23610	-11.23558
-11.23502	-11.23419	-11.23368	-11.23339	-11.23331	-11.22838
-11.21886	-1.39273	-1.26891	-1.16835	-1.14895	-1.10746
-1.03263	-1.02095	-1.01909	-1.01574	-0.95795	-0.94005
-0.85742	-0.84770	-0.83275	-0.82952	-0.78999	-0.74180
-0.71170	-0.69828	-0.66969	-0.66178	-0.64782	-0.63572
-0.63366	-0.61767	-0.61076	-0.60168	-0.60072	-0.58739
-0.57729	-0.56657	-0.55182	-0.54713	-0.52448	-0.52147
-0.51810	-0.51169	-0.50434	-0.49280	-0.48279	-0.47643
-0.46694	-0.41994	-0.40882	-0.34106	-0.33688	-0.32821
-0.30100	0.12978	0.13503	0.13994	0.14887	0.20594
0.23335	0.24132	0.25597	0.26421	0.26853	

end of program scf

start of program der1a
end of program der1a

start of program rwr
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	H1	-5.296982E-05	-3.951173E-04	7.411375E-05
2	C1	9.907697E-05	5.407540E-04	1.234864E-04
3	C2	-4.717926E-05	-1.038051E-04	-7.144838E-04
4	C3	1.761000E-04	-8.715255E-05	1.264820E-04
5	C4	7.962032E-05	3.446371E-04	5.289804E-04
6	C5	3.196140E-05	-8.469596E-04	-9.089075E-04
7	C6	-8.559902E-04	-1.294815E-04	-4.306339E-04
8	C7	-2.515919E-04	-1.448884E-04	2.158885E-05
9	H3	4.533722E-05	-3.383463E-05	2.160514E-04
10	H4	-2.257503E-05	5.991930E-04	6.148878E-05
11	H6	-7.920108E-05	9.247325E-05	4.246163E-04
12	H7	2.873300E-04	5.025521E-05	-4.988166E-05
13	C10	1.480745E-04	-9.282448E-05	3.203226E-05
14	C8	2.184431E-04	2.449099E-04	-1.832425E-04
15	C17	7.505695E-04	3.371929E-04	3.208913E-04
16	N2	1.962310E-03	-3.808634E-03	3.466456E-04
17	C9	-7.788159E-04	-9.254854E-04	4.562717E-03
18	C16	-1.139246E-03	-2.252224E-03	2.057309E-03
19	O1	-9.483710E-04	5.475285E-03	-5.834743E-03
20	C11	1.891329E-04	4.917343E-04	5.709381E-04

```
 21    C12    -7.646449E-04   3.179836E-04   3.997883E-05
 22    C13     6.030974E-04  -4.114957E-04  -2.320855E-04
 23    C14     9.963530E-04  -4.596421E-04  -2.908264E-04
 24    C15    -1.000750E-03   4.567750E-04   5.035355E-05
 25    H19     6.333005E-04  -3.328232E-05   1.977137E-04
 26    H20    -5.753543E-04   6.528583E-04   4.036981E-04
 27    H21    -5.898393E-04   1.342095E-04  -1.348524E-04
 28    H22     5.576637E-04  -3.876170E-04  -2.630419E-04
 29    H23    -4.301430E-05  -1.686902E-04  -2.147066E-04
 30    H27    -1.040082E-04   3.774070E-04  -1.041649E-04
 31    H29    -4.820114E-04  -6.134559E-04  -8.335812E-04
 32    H30    -2.328785E-05  -8.258124E-04  -1.169381E-04
 33    H15     7.454160E-05  -1.334916E-04   6.151745E-04
 34    H2      9.815930E-04   1.151536E-03  -9.994230E-04
 35    H5     -7.754705E-04   1.238134E-03  -2.598928E-04
 36    H8      8.357666E-04  -4.888537E-04   1.161865E-04
-----------   -------------  -------------  -------------
   total       1.359512E-04   1.625905E-04  -6.809589E-04

 end of program der1b


 start of program geopt   7

 geometry optimization step  7
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:          -8.2027E-05 .  (  5.0000E-05 )
 gradient maximum:        7.8198E-03 .  (  4.5000E-04 )
 gradient rms:            1.0535E-03 .  (  3.0000E-04 )
 step size:   0.04120  trust radius:   0.30000
 displacement maximum:    1.7489E-02 .  (  1.8000E-03 )
 displacement rms:        3.7302E-03 .  (  1.2000E-03 )
 predicted energy change:    -1.0975E-04    geom step:   4.1201E-
02    full step:   4.1201E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:     1.1760E-03     y:    -1.9126E-03     z:    -1.6634E-03

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -0.2927369916     1.3311009777    -2.0554944921
 C1       -0.1833266911     1.7707818843    -1.0814524423
 C2        0.1267260072     2.9174976644     1.4044586765
```

```
 C3        0.2199683484      0.9732541177     -0.0236541144
 C4       -0.4419431708      3.1248845165     -0.9163891626
 C5       -0.2927540908      3.6913246877      0.3327114767
 C6        0.3956491473      1.5646951980      1.2355835888
 C7        0.5716810068     -0.5008285830     -0.1519816209
 H3       -0.7544811817      3.7194774437     -1.7563785568
 H4       -0.4967947848      4.7362286818      0.4866510049
 H6        0.2396511045      3.3763832975      2.3669312926
 H7        1.6604873235     -0.5470458947     -0.1732229591
 C10       0.0960056906     -1.2192172516     -1.4072948963
 C8        0.1609283529     -1.2414716764      1.1400339486
 C17      -1.3475438917     -1.3720832891      1.4020565381
 N2        0.8827199245      0.7966724416      2.3180833383
 C9        0.7938459386     -0.5732806090      2.3437817460
 C16       1.4184932870      1.4664782474      3.4919541703
 O1        1.1650996617     -1.2188767325      3.2830694681
 C11      -0.7086989041     -2.6654658313     -3.6654603554
 C12       0.9956718872     -2.0168673786     -2.1062975728
 C13      -1.2194682531     -1.1562022581     -1.8664761269
 C14      -1.6169864336     -1.8701667809     -2.9826344184
 C15       0.6005652448     -2.7358403235     -3.2232090427
 H19       2.0184553212     -2.0775116827     -1.7746360536
 H20      -1.9351051178     -0.5373858176     -1.3577621572
 H21      -2.6365974981     -1.8040888398     -3.3205404821
 H22       1.3168670014     -3.3453233708     -3.7449957669
 H23      -1.0194863279     -3.2198166288     -4.5335692514
 H27      -1.8460472255     -0.4080812591      1.3968718944
 H29      -1.8137390329     -2.0016216367      0.6563096060
 H30       0.5853010360     -2.2374801088      1.1180107926
 H15      -1.5013171791     -1.8297001213      2.3719810793
 H2        2.1010121118      2.2509239933      3.1895373516
 H5        1.9420961548      0.7377896051      4.0817194930
 H8        0.6261417945      1.8979367630      4.0942044532

 nuclear repulsion energy.......  1397.135769061 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   7   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.368E-04
 number of canonical orbitals.....          368
 end of program onee


 start of program probe
 end of program probe
```

```
  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
  grid # 3      210    184    183    192    182    183    194
176
  grid # 4      208    327    326    340    327    327    328
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     82     72
94
  grid # 2      118    118    112    107    100     90     80
104
  grid # 3      223    223    207    206    197    174    151
210
  grid # 4      224    223    205    206    341    313    290
391

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     69    110     89     88     87     89
89
  grid # 2       90     78    122     97     95     95     95
97
  grid # 3      175    147    260    184    183    183    183
184
  grid # 4      292    275    456    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     70
69
  grid # 2      112    111    118    118    118    109    109
109
  grid # 3      214    209    223    223    224    215    210
214
  grid # 4      213    205    223    223    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
```

```
  grid # 1       71     71     70     71   2858
  grid # 2      110    111    107    111   3721
  grid # 3      219    216    213    216   7190
  grid # 4      218    213    209    216   9915

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot  1  N  N  1  U  -783.02992975121             6.7E-05  1.0E-03
etot  2  Y  Y  4  M  -783.03035591409  4.3E-04  2.3E-05  3.0E-04
etot  3  Y  Y  4  M  -783.03040783438  5.2E-05  6.2E-06  1.2E-04
etot  4  Y  Y  4  M  -783.03041044265  2.6E-06  3.2E-06  5.4E-05
etot  5  Y  N  4  M  -783.03041266576  2.2E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1397.13576906084
   (E)  Total one-electron terms..... -3838.64016195461
   (I)  Total two-electron terms.....  1658.47398022801
   (L)  Electronic energy..... -2180.16618172660  (E+I)
   (N)  Total energy.............  -783.03041266576  (A+L)

 SCFE: SCF energy: HF    -783.03041266576 hartrees   iterations:
5


 HOMO energy:    -0.30091
 LUMO energy:     0.12998

  Orbital energies:
  -20.52481  -15.60145  -11.34425  -11.28566  -11.25496  -11.25114
  -11.24498  -11.24334  -11.24059  -11.23713  -11.23604  -11.23547
  -11.23492  -11.23399  -11.23361  -11.23331  -11.23317  -11.22825
  -11.21919   -1.39614   -1.26917   -1.16837   -1.14885   -1.10753
   -1.03264   -1.02093   -1.01913   -1.01542   -0.95821   -0.93989
   -0.85729   -0.84730   -0.83260   -0.82929   -0.78973   -0.74176
   -0.71167   -0.69820   -0.66993   -0.66189   -0.64802   -0.63540
   -0.63386   -0.61741   -0.61119   -0.60175   -0.60086   -0.58746
   -0.57739   -0.56653   -0.55209   -0.54726   -0.52499   -0.52127
   -0.51783   -0.51183   -0.50441   -0.49279   -0.48276   -0.47661
   -0.46683   -0.41987   -0.40868   -0.34091   -0.33688   -0.32807
```

```
 -0.30091    0.12998    0.13541    0.14014    0.14911    0.20705
  0.23321    0.24162    0.25601    0.26458    0.26837

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	2.101214E-04	3.252614E-04	5.602618E-04
2	C1	-2.300805E-04	-1.371761E-04	-5.233361E-04
3	C2	-2.758678E-04	-1.259649E-04	-1.035809E-04
4	C3	9.030691E-05	2.294675E-05	-1.023654E-04
5	C4	3.771848E-05	-3.659104E-04	9.334880E-05
6	C5	1.847390E-04	-3.915992E-04	4.778660E-05
7	C6	3.318597E-04	7.579617E-04	7.831273E-05
8	C7	-1.377053E-04	-3.164977E-04	-3.298678E-04
9	H3	7.403856E-05	-1.327962E-04	2.040446E-04
10	H4	1.322487E-05	6.775048E-05	-5.151132E-05
11	H6	-1.457088E-04	1.360164E-04	-1.185368E-04
12	H7	-1.856213E-04	2.138309E-04	-7.383809E-06
13	C10	1.337306E-04	9.025197E-05	2.231704E-04
14	C8	-2.534031E-04	6.301730E-04	-6.767065E-04
15	C17	5.539060E-05	4.547507E-04	-3.759481E-04
16	N2	-7.756083E-04	-2.084795E-03	-2.569069E-03
17	C9	-1.673549E-04	1.946787E-03	-7.848075E-04
18	C16	-3.347044E-04	7.958961E-04	9.146328E-05
19	O1	7.635698E-04	-5.583899E-04	2.096793E-03
20	C11	-2.447097E-04	-2.380383E-04	-4.464844E-04
21	C12	-7.390991E-05	9.576713E-04	1.112732E-03
22	C13	9.473616E-04	4.939673E-04	6.260765E-04
23	C14	-1.208146E-04	-6.187619E-04	-9.002393E-04
24	C15	-4.929269E-04	-2.872204E-04	-6.120755E-04
25	H19	-1.437939E-04	-4.831191E-05	-4.317223E-05
26	H20	-1.643894E-04	9.753956E-05	2.895091E-04
27	H21	7.566510E-05	-4.757896E-05	3.286946E-05
28	H22	8.691339E-05	-1.901553E-04	-2.361522E-04
29	H23	3.272189E-05	2.281349E-05	6.202587E-05
30	H27	8.661891E-05	4.097314E-05	-5.582268E-05
31	H29	-4.043995E-05	-3.213326E-04	-1.993664E-04
32	H30	1.625190E-04	-7.381874E-05	-3.783268E-05

```
 33    H15    -2.602321E-04  -2.659915E-04   4.036648E-04
 34    H2     -8.311658E-05  -1.390267E-04  -1.896087E-04
 35    H5      1.011353E-03  -9.841210E-04   1.071648E-03
 36    H8     -1.043646E-04   4.358583E-04   6.762420E-04
-----------   -------------  -------------  -------------
   total       6.310076E-05   1.629635E-04  -6.939178E-04

 end of program der1b


 start of program geopt   8

 geometry optimization step  8
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:           8.1217E-05 .  (  5.0000E-05 )
 gradient maximum:        2.1973E-03 .  (  4.5000E-04 )
 gradient rms:            5.3128E-04 .  (  3.0000E-04 )
 step size:   0.03582  trust radius:   0.30000
 displacement maximum:    1.1907E-02 .  (  1.8000E-03 )
 displacement rms:        3.2433E-03 .  (  1.2000E-03 )
 predicted energy change:    -4.0291E-05    geom step:   3.5823E-
02    full step:   3.5823E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -5.7836E-04     y:     2.0927E-03     z:     1.2391E-03

 new geometry:
                              angstroms
 atom            x                y                z
 H1       -0.2661560888     1.3331181465    -2.0592768257
 C1       -0.1688073376     1.7714178806    -1.0848911740
 C2        0.1143739422     2.9147078779     1.4044897936
 C3        0.2272977558     0.9738175048    -0.0251374608
 C4       -0.4337196300     3.1232573021    -0.9199784241
 C5       -0.2988960811     3.6877702357     0.3305023053
 C6        0.3928263088     1.5646040078     1.2352954695
 C7        0.5797554837    -0.4999509524    -0.1540293601
 H3       -0.7406612437     3.7183614091    -1.7608638594
 H4       -0.5091848545     4.7318055939     0.4838010268
 H6        0.2158197527     3.3730701323     2.3681071347
 H7        1.6682970562    -0.5447620847    -0.1784553386
 C10       0.0985884297    -1.2168041457    -1.4072442682
 C8        0.1718787321    -1.2423138226     1.1377432425
 C17      -1.3365676819    -1.3846851741     1.3934833880
```

```
  N2        0.8785477159      0.7969033882      2.3181769784
  C9        0.7948216579     -0.5707137946      2.3456213054
  C16       1.4124179402      1.4673748932      3.4946549640
  O1        1.1635892976     -1.2122542184      3.2907615742
  C11      -0.7205226671     -2.6649489011     -3.6619320187
  C12       0.9903614373     -2.0221429836     -2.1058923427
  C13      -1.2162259344     -1.1460379930     -1.8649917194
  C14      -1.6210652361     -1.8613780895     -2.9791304426
  C15       0.5882779616     -2.7421286267     -3.2212669740
  H19       2.0129316468     -2.0906512795     -1.7756748879
  H20      -1.9277240292     -0.5220337161     -1.3552657341
  H21      -2.6413019272     -1.7895485874     -3.3138270318
  H22       1.2997733947     -3.3587823764     -3.7422741539
  H23      -1.0367111890     -3.2203555075     -4.5272697522
  H27      -1.8419199812     -0.4247253003      1.3852798838
  H29      -1.7931442443     -2.0181624588      0.6450319614
  H30       0.6044222355     -2.2354397781      1.1168926004
  H15      -1.4935666450     -1.8439940263      2.3626064099
  H2        2.0961198120      2.2501736707      3.1892934940
  H5        1.9360089494      0.7399702901      4.0883031565
  H8        0.6214226158      1.9026675566      4.0962522762

  nuclear repulsion energy.......  1397.460839396 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   8   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.350E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
  grid # 3      210    184    182    192    182    183    194
176
```

```
  grid # 4      208    327    326    340    327    327    328
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     81     74
94
  grid # 2      118    118    112    106    100     90     80
104
  grid # 3      223    223    207    207    196    174    149
210
  grid # 4      224    223    206    204    341    315    286
390

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     69    110     89     88     87     89
89
  grid # 2       90     79    122     97     95     95     95
97
  grid # 3      176    145    260    184    182    182    183
184
  grid # 4      293    276    456    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     71
69
  grid # 2      112    112    118    118    118    109    109
109
  grid # 3      214    209    223    223    224    215    210
214
  grid # 4      213    205    223    223    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2860
  grid # 2      110    111    106    111   3721
  grid # 3      219    216    213    216   7184
  grid # 4      218    213    209    216   9913

  end of program grid


  start of program rwr
  end of program rwr
```

```
  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS     maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d     total energy     change  change    error

etot  1  N  N  1  U  -783.03005480403           4.6E-05  1.3E-03
etot  2  Y  Y  4  M  -783.03039517462  3.4E-04  2.0E-05  3.9E-04
etot  3  Y  Y  4  M  -783.03043955592  4.4E-05  5.6E-06  9.5E-05
etot  4  Y  Y  4  M  -783.03044228228  2.7E-06  2.5E-06  3.6E-05
etot  5  Y  N  4  M  -783.03044272633  4.4E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1397.46083939577
   (E)  Total one-electron terms..... -3839.28878476771
   (I)  Total two-electron terms.....  1658.79750264561
   (L)  Electronic energy............. -2180.49128212210  (E+I)
   (N)  Total energy.................  -783.03044272633  (A+L)

 SCFE: SCF energy: HF    -783.03044272633 hartrees   iterations:
5


 HOMO energy:    -0.30123
 LUMO energy:     0.12995

  Orbital energies:
  -20.52401  -15.60160  -11.34415  -11.28568  -11.25515  -11.25129
  -11.24498  -11.24336  -11.24082  -11.23697  -11.23606  -11.23551
  -11.23469  -11.23408  -11.23365  -11.23334  -11.23309  -11.22804
  -11.21915   -1.39500   -1.26917   -1.16862   -1.14927   -1.10766
   -1.03286   -1.02101   -1.01916   -1.01568   -0.95828   -0.94002
   -0.85726   -0.84775   -0.83285   -0.82945   -0.78984   -0.74196
   -0.71172   -0.69822   -0.66992   -0.66196   -0.64810   -0.63532
   -0.63395   -0.61757   -0.61106   -0.60143   -0.60093   -0.58699
   -0.57735   -0.56659   -0.55189   -0.54714   -0.52472   -0.52149
   -0.51787   -0.51197   -0.50444   -0.49279   -0.48264   -0.47670
   -0.46695   -0.41981   -0.40856   -0.34103   -0.33682   -0.32824
   -0.30123    0.12995    0.13534    0.14003    0.14916    0.20708
    0.23326    0.24137    0.25581    0.26422    0.26839

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
```

```
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	-1.140719E-04	-6.499710E-05	-4.130554E-04
2	C1	-2.851578E-05	-4.050072E-04	-1.286143E-04
3	C2	9.295780E-06	1.684741E-04	2.062980E-04
4	C3	-9.064331E-06	-2.174090E-04	-3.464953E-05
5	C4	-8.561083E-05	3.278602E-05	-4.057126E-04
6	C5	-2.134558E-05	5.879712E-04	5.337846E-04
7	C6	3.101503E-04	-2.331394E-06	-1.435943E-05
8	C7	1.535559E-04	2.003033E-04	1.097061E-04
9	H3	-4.593092E-05	7.668884E-05	-2.478549E-04
10	H4	2.771560E-05	-1.075377E-04	-9.184986E-06
11	H6	4.185435E-05	1.408314E-04	2.233013E-04
12	H7	-9.688335E-06	1.087746E-06	-6.279909E-05
13	C10	1.681820E-04	-5.778707E-05	-2.853702E-05
14	C8	9.019550E-07	-2.167687E-04	2.607292E-04
15	C17	1.122140E-05	-1.285885E-04	-2.406471E-04
16	N2	-2.639286E-04	-2.339978E-04	-3.244891E-04
17	C9	3.247545E-04	-2.949153E-04	5.711815E-04
18	C16	3.927602E-04	1.061726E-03	-3.868351E-04
19	O1	-2.574556E-04	-7.308353E-05	-5.410925E-04
20	C11	-3.185205E-04	-4.440273E-05	-2.260312E-04
21	C12	2.482342E-04	-1.201203E-04	-5.156046E-05
22	C13	-4.250885E-04	1.552174E-04	-7.201405E-05
23	C14	-3.416585E-04	2.508047E-04	1.510462E-04
24	C15	6.219917E-04	-1.219123E-04	1.325961E-04
25	H19	2.639330E-05	-3.705209E-06	-3.293485E-05
26	H20	1.417312E-04	-2.163832E-04	-1.403268E-04
27	H21	3.022227E-05	-1.428976E-05	-1.563539E-05
28	H22	-5.346949E-05	8.191457E-05	2.455726E-06
29	H23	-1.566653E-05	2.710134E-05	-2.446166E-05
30	H27	-1.150750E-04	2.778667E-04	-4.094068E-05
31	H29	-1.847337E-04	-1.529253E-04	-1.316522E-04
32	H30	-8.930115E-05	1.707525E-04	-4.601085E-05
33	H15	5.792980E-05	-9.170692E-05	1.736207E-04
34	H2	-2.270907E-04	-1.396650E-04	1.421172E-04
35	H5	3.937866E-04	-5.005298E-04	1.826675E-04
36	H8	-2.948098E-04	1.257423E-04	2.844157E-04
total		5.965533E-05	1.512038E-04	-6.454795E-04

```
 end of program der1b


 start of program geopt   9
```

```
  geometry optimization step  9
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -3.0061E-05 *  (  5.0000E-05 )
  gradient maximum:        9.0408E-04 .  (  4.5000E-04 )
  gradient rms:            2.4230E-04 *  (  3.0000E-04 )
  step size:   0.02715  trust radius:   0.30000
  displacement maximum:    1.2180E-02 .  (  1.8000E-03 )
  displacement rms:        2.4579E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.6126E-05    geom step:   2.7148E-
02    full step:   2.7148E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -6.5958E-04     y:    -6.2602E-04     z:    -2.0780E-06

  new geometry:
                                angstroms
  atom            x                 y                 z
  H1       -0.2845459323     1.3327285376     -2.0573909308
  C1       -0.1791008872     1.7710185966     -1.0833420858
  C2        0.1225454738     2.9171311114      1.4058355007
  C3        0.2236889338     0.9744914765     -0.0248506210
  C4       -0.4400315388     3.1238724854     -0.9170333148
  C5       -0.2951211177     3.6899492554      0.3331003911
  C6        0.3969821060     1.5661562567      1.2351359488
  C7        0.5752451540    -0.4996287496     -0.1527233951
  H3       -0.7513549306     3.7188825381     -1.7568353852
  H4       -0.5020404945     4.7344702084      0.4863286551
  H6        0.2299078119     3.3757016952      2.3691174654
  H7        1.6637488241    -0.5447830002     -0.1737145261
  C10       0.0989032950    -1.2174709565     -1.4073854817
  C8        0.1625917402    -1.2402383746      1.1388865746
  C17      -1.3470644543    -1.3761641938      1.3938161122
  N2        0.8819640704     0.7964269836      2.3170890667
  C9        0.7900545487    -0.5713921018      2.3463689878
  C16       1.4232201306     1.4647665998      3.4919994935
  O1        1.1551447010    -1.2152808126      3.2909700228
  C11      -0.7114608759    -2.6679524120     -3.6646747001
  C12       0.9957018191    -2.0174325861     -2.1061914853
  C13      -1.2162366752    -1.1532749195     -1.8662379779
  C14      -1.6169526257    -1.8697342124     -2.9815093851
  C15       0.5981527328    -2.7386557135     -3.2228999547
  H19       2.0184309175    -2.0808859242     -1.7753024949
  H20      -1.9315851677    -0.5345993739     -1.3561507383
```

```
  H21      -2.6373787535     -1.8035444899     -3.3164776368
  H22       1.3131853908     -3.3508233606     -3.7443086476
  H23      -1.0240737839     -3.2241848300     -4.5307086589
  H27      -1.8490136671     -0.4141691570      1.3810350438
  H29      -1.8059030876     -2.0116903425      0.6484031489
  H30       0.5903930159     -2.2350250948      1.1182690951
  H15      -1.5058138117     -1.8305676362      2.3651251224
  H2        2.1004048377      2.2514094317      3.1845141854
  H5        1.9560113846      0.7352964011      4.0778796517
  H8        0.6353235099      1.8943286149      4.1027977401

  nuclear repulsion energy.......  1397.070099237 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration   9   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.367E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
  grid # 3      210    184    182    192    182    183    190
176
  grid # 4      208    327    326    340    327    327    327
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     82     74
94
  grid # 2      118    118    112    106    100     90     80
104
  grid # 3      223    223    207    207    196    174    149
211
```

```
  grid # 4      224    223    206    204    341    314    287
390

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     71    110     89     88     87     89
89
  grid # 2       91     79    122     97     95     95     95
97
  grid # 3      176    142    260    184    182    182    183
184
  grid # 4      293    273    456    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     71
69
  grid # 2      112    111    118    118    118    110    109
109
  grid # 3      214    209    223    223    224    215    210
214
  grid # 4      213    205    223    223    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2863
  grid # 2      110    111    107    111   3723
  grid # 3      219    215    212    216   7176
  grid # 4      218    213    209    218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

      i  u  d  i  g                                          RMS    maximum
      t  p  i  c  r                                 energy density   DIIS
      e  d  i  u  i                 total energy    change change    error

etot  1  N  N  1  U  -783.03024646847                3.6E-05  7.3E-04
etot  2  Y  Y  4  M  -783.03044494347  2.0E-04  1.5E-05  2.7E-04
etot  3  Y  Y  4  M  -783.03047014621  2.5E-05  4.3E-06  6.8E-05
etot  4  Y  N  4  M  -783.03047351487  3.4E-06  0.0E+00  0.0E+00
```

```
 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1397.07009923731
   (E)  Total one-electron terms..... -3838.50925197305
   (I)  Total two-electron terms.....  1658.40867922087
   (L)  Electronic energy..... -2180.10057275218  (E+I)
   (N)  Total energy.............  -783.03047351487  (A+L)

 SCFE: SCF energy: HF    -783.03047351487 hartrees   iterations:
4


 HOMO energy:    -0.30109
 LUMO energy:     0.12987

  Orbital energies:
 -20.52409  -15.60182  -11.34430  -11.28593  -11.25554  -11.25118
 -11.24500  -11.24355  -11.24076  -11.23722  -11.23620  -11.23573
 -11.23485  -11.23421  -11.23374  -11.23351  -11.23335  -11.22834
 -11.21926   -1.39511   -1.26909   -1.16836   -1.14896   -1.10744
  -1.03264   -1.02085   -1.01896   -1.01563   -0.95810   -0.93993
  -0.85719   -0.84761   -0.83273   -0.82942   -0.78970   -0.74191
  -0.71159   -0.69811   -0.66977   -0.66194   -0.64796   -0.63535
  -0.63374   -0.61765   -0.61099   -0.60143   -0.60084   -0.58700
  -0.57723   -0.56654   -0.55190   -0.54725   -0.52461   -0.52139
  -0.51780   -0.51189   -0.50437   -0.49276   -0.48266   -0.47660
  -0.46691   -0.41982   -0.40854   -0.34091   -0.33677   -0.32831
  -0.30109    0.12987    0.13524    0.14002    0.14898    0.20694
   0.23321    0.24147    0.25593    0.26462    0.26840

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x             y             z
 ----  -----   -------------  ------------  ------------
   1    H1      4.306824E-05  -3.811675E-05  -5.825168E-05
   2    C1      1.154014E-04  -1.090558E-05   2.597666E-04
   3    C2     -2.381388E-05  -2.507239E-05  -2.212867E-04
   4    C3      9.454534E-05   7.093486E-05   2.691954E-04
```

5	C4	4.834871E-05	3.249837E-04	4.060106E-04
6	C5	-1.032731E-04	-1.014322E-04	-4.532629E-04
7	C6	-2.328858E-04	-3.086883E-04	-3.900162E-04
8	C7	-1.462801E-04	1.273884E-04	1.398661E-04
9	H3	1.602115E-05	2.841850E-05	2.775624E-05
10	H4	-2.432367E-05	3.481805E-05	-2.075562E-05
11	H6	-4.323444E-05	2.896488E-05	-1.703978E-05
12	H7	6.452597E-05	-3.158282E-05	1.821965E-05
13	C10	-7.185283E-05	-5.402895E-05	-1.061039E-04
14	C8	-2.362070E-05	-4.724389E-06	1.939075E-05
15	C17	2.182348E-04	1.251015E-04	-2.401046E-05
16	N2	1.404209E-04	-5.991710E-04	-1.276636E-04
17	C9	-2.381548E-04	2.199369E-04	-1.705079E-04
18	C16	2.797178E-04	-2.077793E-04	3.107259E-04
19	O1	3.181108E-06	1.856006E-04	-6.758988E-05
20	C11	2.096776E-04	1.394250E-04	2.408279E-04
21	C12	-1.596296E-05	-2.569227E-04	-3.510612E-04
22	C13	-1.555350E-04	-1.672252E-04	-2.707349E-04
23	C14	1.964782E-04	1.144488E-04	2.075390E-04
24	C15	-4.103885E-05	1.724779E-04	1.811446E-04
25	H19	-1.160934E-05	-1.327539E-05	-2.394384E-05
26	H20	9.037253E-06	3.748885E-05	-2.523035E-05
27	H21	-3.523915E-05	4.616328E-05	-4.226316E-05
28	H22	-4.454817E-05	5.171548E-05	3.861588E-05
29	H23	-1.309298E-05	-2.408279E-06	-4.697281E-05
30	H27	-3.013976E-05	8.969003E-05	-8.863575E-06
31	H29	-7.378555E-05	-1.168342E-04	-1.709723E-04
32	H30	3.576530E-05	-9.268952E-05	-4.069871E-05
33	H15	1.263289E-05	-5.484992E-05	8.593593E-05
34	H2	1.130454E-04	8.140374E-05	-5.315252E-05
35	H5	-2.243693E-04	4.003631E-04	-2.607665E-04
36	H8	7.983436E-06	-8.861580E-05	1.016309E-04
total		5.532520E-05	1.050009E-04	-6.445230E-04

```
 end of program der1b


 start of program geopt  10

 geometry optimization step 10
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:          -3.0789E-05 *  (  5.0000E-05 )
 gradient maximum:        6.1013E-04 .  (  4.5000E-04 )
```

```
  gradient rms:            1.6032E-04 *  (  3.0000E-04 )
  step size:   0.01877  trust radius:   0.30000
  displacement maximum:    9.6422E-03 .  (  1.8000E-03 )
  displacement rms:        1.6998E-03 .  (  1.2000E-03 )
  predicted energy change:    -6.8349E-06    geom step:   1.8774E-
02    full step:   1.8774E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.2012E-03     y:    -1.4607E-04     z:     8.2086E-04

  new geometry:
                              angstroms
  atom            x                y                z
  H1       -0.2801543114     1.3334031349    -2.0579415504
  C1       -0.1773871749     1.7709961548    -1.0832454970
  C2        0.1183331768     2.9157085117     1.4061249142
  C3        0.2242652863     0.9738403944    -0.0248605939
  C4       -0.4408983669     3.1237910147    -0.9165815708
  C5       -0.2998914169     3.6890991827     0.3337062967
  C6        0.3958946367     1.5651902243     1.2347353089
  C7        0.5753391405    -0.5003085386    -0.1517533413
  H3       -0.7518253429     3.7188308819    -1.7565228357
  H4       -0.5097039619     4.7329266499     0.4875830200
  H6        0.2233746455     3.3733273418     2.3701328921
  H7        1.6639408297    -0.5462687834    -0.1714735003
  C10       0.0998016674    -1.2181940707    -1.4068119488
  C8        0.1609701441    -1.2406582233     1.1395300575
  C17      -1.3487745999    -1.3762300464     1.3926738477
  N2        0.8836146097     0.7959701849     2.3160845117
  C9        0.7873338416    -0.5713047834     2.3470856196
  C16       1.4317218732     1.4658409070     3.4869806224
  O1        1.1490238845    -1.2143882872     3.2936240933
  C11      -0.7087473416    -2.6658374689    -3.6648149368
  C12       0.9963301689    -2.0205698466    -2.1032878318
  C13      -1.2143015298    -1.1508741226    -1.8679620183
  C14      -1.6140131067    -1.8656875482    -2.9838323267
  C15       0.5994372277    -2.7402921776    -3.2203892798
  H19       2.0179962640    -2.0866416941    -1.7700863618
  H20      -1.9289457993    -0.5304540149    -1.3592368761
  H21      -2.6333247730    -1.7966137199    -3.3216034819
  H22       1.3136726773    -3.3541738717    -3.7403794318
  H23      -1.0208274086    -3.2208277852    -4.5319016378
  H27      -1.8502918483    -0.4137753301     1.3818308739
  H29      -1.8077854758    -2.0100637773     0.6456422032
  H30       0.5887680650    -2.2355639401     1.1195584936
  H15      -1.5079703611    -1.8326702903     2.3630581178
  H2        2.1019451466     2.2563966645     3.1749556526
  H5        1.9731916045     0.7384401749     4.0668056839
  H8        0.6466945871     1.8895516239     4.1058699479

  nuclear repulsion energy.......  1397.194479648 hartrees
```

```
  ------------------------------------------------
 /  end of geometry optimization iteration  10   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.365E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
  grid # 3      210    184    182    192    182    183    194
176
  grid # 4      208    327    327    340    327    327    328
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     82     74
94
  grid # 2      118    118    112    106    100     90     80
104
  grid # 3      223    223    207    207    196    174    149
210
  grid # 4      224    223    206    204    341    313    287
390

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     71    110     89     88     87     89
89
  grid # 2       91     79    122     97     95     95     95
97
  grid # 3      176    140    260    184    183    182    183
184
```

```
  grid # 4      293    271    456    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     71
69
  grid # 2      112    111    118    118    118    109    109
109
  grid # 3      214    209    223    223    224    215    210
214
  grid # 4      213    205    223    223    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2863
  grid # 2      110    111    108    111   3723
  grid # 3      219    215    212    216   7178
  grid # 4      218    213    209    218   9910

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                              RMS    maximum
       t  p  i  c  r                                 energy  density   DIIS
       e  d  i  u  i                                 change  change    error
       r  t  s  t  d     total energy

etot   1  N  N  1  U  -783.03038833871                        2.8E-05  5.9E-04
etot   2  Y  Y  4  M  -783.03046554246  7.7E-05  1.0E-05  1.9E-04
etot   3  Y  Y  4  M  -783.03047618726  1.1E-05  2.7E-06  4.4E-05
etot   4  Y  N  4  M  -783.03047632766  1.4E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1397.19447964800
   (E)  Total one-electron terms..... -3838.76211632937
   (I)  Total two-electron terms.....  1658.53716035371
   (L)  Electronic energy............. -2180.22495597566  (E+I)
   (N)  Total energy.................  -783.03047632766  (A+L)

 SCFE: SCF energy: HF    -783.03047632766 hartrees   iterations:
4
```

```
HOMO energy:    -0.30118
LUMO energy:     0.12992

 Orbital energies:
 -20.52437  -15.60145  -11.34407  -11.28562  -11.25549  -11.25121
 -11.24504  -11.24339  -11.24074  -11.23716  -11.23605  -11.23550
 -11.23494  -11.23403  -11.23364  -11.23340  -11.23334  -11.22831
 -11.21925   -1.39505   -1.26893   -1.16844   -1.14899   -1.10746
  -1.03264   -1.02094   -1.01903   -1.01553   -0.95810   -0.93990
  -0.85720   -0.84745   -0.83282   -0.82939   -0.78974   -0.74183
  -0.71160   -0.69815   -0.66970   -0.66198   -0.64792   -0.63529
  -0.63380   -0.61757   -0.61093   -0.60134   -0.60085   -0.58715
  -0.57719   -0.56654   -0.55176   -0.54747   -0.52450   -0.52137
  -0.51774   -0.51184   -0.50443   -0.49277   -0.48258   -0.47663
  -0.46696   -0.41962   -0.40859   -0.34095   -0.33683   -0.32821
  -0.30118    0.12992    0.13539    0.14006    0.14902    0.20690
   0.23325    0.24135    0.25589    0.26424    0.26844

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H1     -3.512119E-05  -7.246920E-06   1.220435E-05
  2    C1     -6.548342E-05   2.609361E-04   1.161988E-05
  3    C2     -2.424057E-05  -7.665663E-05  -1.612234E-04
  4    C3     -1.799699E-05   5.606370E-05  -1.016539E-04
  5    C4      2.362726E-05  -2.397678E-04  -1.116338E-04
  6    C5      1.206175E-04  -2.094980E-04   1.366455E-04
  7    C6     -5.770954E-05   2.534923E-04   1.086819E-04
  8    C7      1.516521E-05  -7.941797E-05  -7.151312E-05
  9    H3      2.135461E-05  -4.442957E-05   9.021892E-06
 10    H4      2.587308E-05   2.607905E-05   6.297830E-06
 11    H6      3.342028E-06   1.970645E-05  -6.520183E-06
 12    H7     -2.218596E-05   3.905096E-06   1.303655E-05
 13    C10     7.462964E-05   4.586939E-05   9.724657E-05
 14    C8     -5.899785E-05   1.013763E-04  -1.928770E-04
 15    C17     2.495023E-05   5.634245E-05   3.962970E-05
 16    N2      1.293758E-05  -5.234874E-05  -6.473087E-04
```

```
  17    C9     -3.117297E-05   7.077924E-05   5.248981E-04
  18    C16    -1.426884E-04  -4.703364E-04   4.721695E-04
  19    O1      9.020199E-05   1.939353E-04  -1.792002E-04
  20    C11    -1.303666E-04  -2.800319E-05  -1.342712E-04
  21    C12    -3.136288E-05   1.545941E-04   1.150223E-04
  22    C13     8.039724E-05   7.889090E-05   1.099894E-04
  23    C14    -5.661729E-05  -1.273047E-04  -1.679750E-04
  24    C15    -3.412673E-05  -4.641936E-05  -1.093122E-04
  25    H19     7.235128E-05   3.372425E-05  -7.624453E-06
  26    H20    -2.998671E-05   3.856401E-05   1.677321E-05
  27    H21    -2.573116E-05  -2.035721E-05  -1.544941E-05
  28    H22     7.803951E-05  -3.806013E-05  -7.179592E-05
  29    H23     7.255008E-06  -5.960961E-06  -1.590225E-05
  30    H27     2.668901E-05  -2.638931E-05  -3.123892E-05
  31    H29     1.934055E-05  -2.333623E-05  -6.392963E-05
  32    H30     3.277204E-06   3.448445E-06  -1.458692E-05
  33    H15    -3.669980E-05  -2.993639E-06   1.828401E-05
  34    H2      7.682034E-05   7.300693E-05  -1.580492E-04
  35    H5     -7.127518E-05   1.969056E-04  -3.648505E-05
  36    H8      1.573509E-04  -4.120966E-05   2.512862E-05
 -----------   -------------  -------------  -------------
    total       6.245689E-05   1.278832E-04  -5.819011E-04

  end of program der1b


  start of program geopt  11

  geometry optimization step 11
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -2.8128E-06 *  (  5.0000E-05 )
  gradient maximum:        7.7316E-04 .  (  4.5000E-04 )
  gradient rms:            1.3555E-04 *  (  3.0000E-04 )
  step size:   0.01100  trust radius:   0.30000
  displacement maximum:    5.1788E-03 .  (  1.8000E-03 )
  displacement rms:        9.9554E-04 *  (  1.2000E-03 )
  predicted energy change:    -2.9763E-06    geom step:   1.0996E-
02    full step:   1.0996E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -4.5574E-04     y:    -1.0654E-04     z:     7.8232E-05

  new geometry:
                                angstroms
```

```
 atom            x                   y                   z
 H1       -0.2843289727       1.3317189557      -2.0568729495
 C1       -0.1792387241       1.7701933000      -1.0827450722
 C2        0.1206764819       2.9158366153       1.4054453447
 C3        0.2229868296       0.9734199978      -0.0245926193
 C4       -0.4403319880       3.1232905190      -0.9165869976
 C5       -0.2970107617       3.6890672896       0.3330965817
 C6        0.3962817155       1.5651603773       1.2344677208
 C7        0.5733491443      -0.5009564457      -0.1506574137
 H3       -0.7511030611       3.7182273727      -1.7564691967
 H4       -0.5046792615       4.7334138532       0.4866416998
 H6        0.2270802107       3.3737910064       2.3691650567
 H7        1.6620016195      -0.5475384785      -0.1687967207
 C10       0.0993127442      -1.2186173517      -1.4064030227
 C8        0.1577952251      -1.2404147689       1.1407182957
 C17      -1.3519476873      -1.3743776161       1.3940433078
 N2        0.8848395004       0.7957366112       2.3150219486
 C9        0.7850523487      -0.5710000336       2.3480024134
 C16       1.4343437848       1.4645203079       3.4859459816
 O1        1.1458934467      -1.2134966867       3.2951502278
 C11      -0.7060326725      -2.6657445392      -3.6660517259
 C12       0.9981694769      -2.0167225983      -2.1049050565
 C13      -1.2153435861      -1.1545897420      -1.8669724021
 C14      -1.6135006268      -1.8694794897      -2.9834556136
 C15       0.6028759367      -2.7362018523      -3.2227403487
 H19       2.0204887773      -2.0793053919      -1.7726969516
 H20      -1.9314777646      -0.5365077904      -1.3574488212
 H21      -2.6332735899      -1.8033326856      -3.3205317681
 H22       1.3190145421      -3.3467214040      -3.7441591024
 H23      -1.0168442783      -3.2207620646      -4.5336062478
 H27      -1.8527613926      -0.4116203612       1.3810790398
 H29      -1.8112046867      -2.0095505426       0.6480486027
 H30       0.5846336660      -2.2357752810       1.1212978228
 H15      -1.5118139158      -1.8287762158       2.3653913084
 H2        2.1030823104       2.2562734416       3.1726770859
 H5        1.9780017886       0.7381231964       4.0641617571
 H8        0.6505022089       1.8866629125       4.1071446409

 nuclear repulsion energy.......  1397.203718552 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  11   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    3.362E-04
 number of canonical orbitals.....          368
 end of program onee
```

```
  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
  grid # 3      210    184    182    192    182    183    194
176
  grid # 4      208    327    326    340    327    327    328
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     82     73
94
  grid # 2      118    118    112    106    100     90     80
104
  grid # 3      223    223    207    207    196    174    147
210
  grid # 4      224    223    206    204    341    314    287
390

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     71    110     89     88     87     89
89
  grid # 2       91     79    122     97     95     95     95
97
  grid # 3      176    142    260    184    183    183    183
184
  grid # 4      293    272    456    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     70
69
  grid # 2      112    111    118    118    118    110    109
109
  grid # 3      214    209    223    223    224    215    210
214
```

```
  grid # 4      213    205    223    223    224    212    207
208

  number of gridpoints:
     atom       H15     H2      H5      H8  total
  grid # 1       71     71      70      71   2861
  grid # 2      110    111     108     111   3724
  grid # 3      219    215     212     216   7179
  grid # 4      218    213     209     218   9911

  end of program grid


  start of program rwr
  end of program rwr


  start of program scf

       i  u  d  i  g                                          RMS     maximum
       t  p  i  c  r                              energy   density    DIIS
       e  d  i  u  i                              change   change     error
       r  t  s  t  d     total energy

etot   1  N  N  1  U  -783.03043154471                      2.2E-05  4.7E-04
etot   2  Y  Y  4  M  -783.03046609900  3.5E-05  7.1E-06  1.7E-04
etot   3  Y  Y  4  M  -783.03046988043  3.8E-06  2.0E-06  4.4E-05
etot   4  Y  N  4  M  -783.03046921457 -6.7E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1397.20371855239
   (E)  Total one-electron terms..... -3838.77789086563
   (I)  Total two-electron terms.....  1658.54370309866
   (L)  Electronic energy............. -2180.23418776696  (E+I)
   (N)  Total energy.................  -783.03046921457  (A+L)

 SCFE: SCF energy: HF    -783.03046921457 hartrees   iterations:
4


 HOMO energy:    -0.30123
 LUMO energy:     0.12991

  Orbital energies:
  -20.52397  -15.60166  -11.34416  -11.28573  -11.25548  -11.25124
  -11.24501  -11.24343  -11.24082  -11.23705  -11.23609  -11.23560
  -11.23479  -11.23409  -11.23371  -11.23339  -11.23331  -11.22818
  -11.21930   -1.39508   -1.26910   -1.16844   -1.14908   -1.10751
   -1.03268   -1.02096   -1.01908   -1.01560   -0.95817   -0.93994
   -0.85719   -0.84753   -0.83285   -0.82942   -0.78975   -0.74192
   -0.71162   -0.69815   -0.66969   -0.66207   -0.64797   -0.63530
```

```
 -0.63381   -0.61757   -0.61096   -0.60127   -0.60089   -0.58716
 -0.57720   -0.56657   -0.55176   -0.54753   -0.52449   -0.52141
 -0.51774   -0.51191   -0.50439   -0.49276   -0.48256   -0.47666
 -0.46701   -0.41967   -0.40853   -0.34095   -0.33683   -0.32826
 -0.30123    0.12991    0.13542    0.14007    0.14899    0.20690
  0.23319    0.24138    0.25589    0.26427    0.26844

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	1.802924E-05	5.805059E-05	-5.077942E-06
2	C1	-5.960102E-05	3.324249E-06	-1.877636E-04
3	C2	3.019237E-05	-5.855272E-05	1.265697E-04
4	C3	3.254628E-05	-5.762696E-05	1.905349E-05
5	C4	-2.754577E-05	-1.275420E-04	-1.629250E-04
6	C5	-2.928863E-06	9.821992E-05	6.909518E-05
7	C6	8.424220E-05	1.100294E-04	2.494659E-05
8	C7	5.741945E-05	-5.679208E-05	-7.667695E-05
9	H3	-3.089983E-05	4.204100E-05	-8.689056E-05
10	H4	-1.810447E-05	1.096620E-05	-1.748854E-05
11	H6	-4.647679E-06	2.245233E-05	9.499923E-07
12	H7	-6.181147E-05	4.130818E-05	-3.556904E-05
13	C10	4.811207E-06	4.695883E-05	2.265063E-05
14	C8	-3.492065E-06	6.211586E-05	2.811034E-06
15	C17	-7.034161E-05	-7.373710E-05	-2.632369E-05
16	N2	-1.949746E-05	-1.505710E-04	-1.775892E-04
17	C9	-1.904806E-07	4.626478E-05	4.826847E-05
18	C16	4.128959E-06	1.276065E-04	7.379912E-05
19	O1	1.351325E-05	-1.279618E-05	-2.769558E-05
20	C11	1.028080E-06	-5.370811E-05	-9.671318E-05
21	C12	-4.066874E-05	1.335075E-04	1.601364E-04
22	C13	1.870173E-04	5.787544E-05	1.029179E-04
23	C14	-2.024104E-05	-5.409904E-05	-1.467137E-04
24	C15	-8.992304E-05	-5.013730E-05	-1.248842E-04
25	H19	-1.858326E-05	-2.385863E-05	-8.764175E-06
26	H20	-2.872420E-05	3.644373E-05	2.117903E-05
27	H21	-4.763134E-06	1.364255E-05	-2.766448E-05
28	H22	2.681378E-05	-5.058570E-05	-5.285894E-05

```
 29    H23     8.141049E-06   7.852019E-06  -1.009039E-05
 30    H27     3.835170E-06  -1.418811E-05  -2.088234E-05
 31    H29     2.308237E-05   3.742999E-05   2.359027E-05
 32    H30     5.815828E-06   2.777707E-07  -2.336051E-05
 33    H15    -1.297210E-05   1.502290E-05  -4.766110E-05
 34    H2     -6.307626E-05  -4.772271E-05  -7.778354E-07
 35    H5      1.100550E-04  -1.093342E-04   4.771365E-05
 36    H8      2.857553E-05   3.425513E-05   3.818034E-05
-----------   -------------  -------------  -------------
   total       6.123460E-05   6.439293E-05  -5.825094E-04

 end of program der1b


 start of program geopt  12

 geometry optimization step 12
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format


 energy change:           7.1131E-06 *  (  5.0000E-05 )
 gradient maximum:        2.5751E-04 *  (  4.5000E-04 )
 gradient rms:            8.2541E-05 *  (  3.0000E-04 )
 step size:   0.01040  trust radius:   0.30000
 displacement maximum:    4.7711E-03 .  (  1.8000E-03 )
 displacement rms:        9.4146E-04 *  (  1.2000E-03 )
 predicted energy change:    -1.9758E-06    geom step:   1.0399E-
02    full step:   1.0399E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:    -2.9823E-04     y:     1.5662E-04     z:     1.7481E-05

 new geometry:
                                angstroms
 atom            x                 y                 z
 H1       -0.2888469178      1.3336875735     -2.0563528799
 C1       -0.1826088041      1.7714963081     -1.0820807793
 C2        0.1210101070      2.9159260429      1.4069493971
 C3        0.2220891920      0.9746121353     -0.0246497933
 C4       -0.4445529615      3.1240220324     -0.9147162753
 C5       -0.2992847690      3.6891527640      0.3353636715
 C6        0.3972877766      1.5658560941      1.2346348561
 C7        0.5724637974     -0.4998087279     -0.1509217160
 H3       -0.7574530211      3.7192870532     -1.7538012569
 H4       -0.5078395944      4.7332516039      0.4897122237
 H6        0.2285263218      3.3733796141      2.3708674379
 H7        1.6610043180     -0.5461132402     -0.1681763113
 C10       0.0996664997     -1.2179441528     -1.4066538220
```

```
  C8        0.1557075276     -1.2390408567      1.1402279300
  C17      -1.3543203040     -1.3718269453      1.3928672658
  N2        0.8877093494      0.7955144879      2.3137767970
  C9        0.7838769053     -0.5707873750      2.3477329037
  C16       1.4400379180      1.4622473192      3.4846465068
  O1        1.1435095937     -1.2137132613      3.2948186721
  C11      -0.7031535449     -2.6684073366     -3.6662255175
  C12       0.9985732118     -2.0184164428     -2.1023476404
  C13      -1.2138999209     -1.1534340226     -1.8698038217
  C14      -1.6107861530     -1.8698031420     -2.9863708228
  C15       0.6046676707     -2.7396282884     -3.2200883295
  H19       2.0201525407     -2.0821704176     -1.7679210621
  H20      -1.9306684938     -0.5340689467     -1.3623185628
  H21      -2.6299550820     -1.8029487434     -3.3253123090
  H22       1.3212999336     -3.3522206553     -3.7388175324
  H23      -1.0129371915     -3.2246072710     -4.5333718478
  H27      -1.8545109342     -0.4088370770      1.3789510031
  H29      -1.8134240560     -2.0068722202      0.6467807049
  H30       0.5815417810     -2.2348314475      1.1207308771
  H15      -1.5152587625     -1.8255754651      2.3642365784
  H2        2.1056102265      2.2560944599      3.1698747533
  H5        1.9877959242      0.7357324650      4.0591543802
  H8        0.6581400897      1.8817569205      4.1100780995

  nuclear repulsion energy.......  1397.147934322 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  12   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.364E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
```

```
  grid # 3      210    184    182    192    182    183    192
176
  grid # 4      208    327    326    340    327    327    327
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     82     74
94
  grid # 2      118    118    112    106    100     90     80
104
  grid # 3      223    223    207    207    196    174    147
211
  grid # 4      224    223    206    204    341    314    285
390

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     71    110     89     88     87     89
89
  grid # 2       91     79    122     97     95     95     95
97
  grid # 3      176    142    260    184    182    182    183
184
  grid # 4      293    272    456    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     71
69
  grid # 2      112    111    118    118    118    110    109
109
  grid # 3      214    209    223    223    224    215    210
214
  grid # 4      213    205    223    223    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2863
  grid # 2      110    111    108    111   3724
  grid # 3      219    215    212    217   7177
  grid # 4      218    213    209    218   9908

  end of program grid


  start of program rwr
```

```
 recomputing RwR matrix  16    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS     maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error

etot   1  N  N  1  U  -783.03046880242           2.5E-05  2.9E-04
etot   2  Y  Y  4  M  -783.03050108369  3.2E-05  6.3E-06  1.1E-04
etot   3  Y  Y  4  M  -783.03050613291  5.0E-06  2.4E-06  3.4E-05
etot   4  Y  N  4  M  -783.03050627684  1.4E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.............  1397.14793432183
   (E)  Total one-electron terms..... -3838.66971023152
   (I)  Total two-electron terms.....  1658.49126963285
   (L)  Electronic energy............. -2180.17844059866  (E+I)
   (N)  Total energy.................  -783.03050627684  (A+L)

 SCFE: SCF energy: HF    -783.03050627684 hartrees   iterations:
4


 HOMO energy:    -0.30123
 LUMO energy:     0.12995

  Orbital energies:
  -20.52431  -15.60133  -11.34393  -11.28553  -11.25549  -11.25112
  -11.24498  -11.24342  -11.24066  -11.23722  -11.23621  -11.23563
  -11.23489  -11.23416  -11.23374  -11.23345  -11.23336  -11.22835
  -11.21922   -1.39523   -1.26895   -1.16837   -1.14903   -1.10742
   -1.03260   -1.02085   -1.01903   -1.01563   -0.95806   -0.93990
   -0.85714   -0.84746   -0.83283   -0.82939   -0.78968   -0.74190
   -0.71156   -0.69809   -0.66967   -0.66205   -0.64794   -0.63524
   -0.63374   -0.61766   -0.61097   -0.60121   -0.60086   -0.58701
   -0.57714   -0.56653   -0.55179   -0.54758   -0.52446   -0.52139
   -0.51766   -0.51188   -0.50440   -0.49274   -0.48255   -0.47665
   -0.46694   -0.41964   -0.40856   -0.34089   -0.33675   -0.32833
   -0.30123    0.12995    0.13538    0.14003    0.14900    0.20694
    0.23319    0.24137    0.25594    0.26432    0.26848

  end of program scf


  start of program der1a
  end of program der1a
```

```
 start of program rwr
recomputing RwR matrix  16    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	H1	1.979650E-05	-2.125731E-06	2.213030E-05
2	C1	5.386030E-05	-2.347237E-04	2.981331E-06
3	C2	-4.508377E-05	1.798364E-04	-2.923902E-05
4	C3	1.894356E-05	-6.997009E-05	-1.000931E-05
5	C4	-1.764153E-06	2.161340E-04	1.366070E-04
6	C5	-3.957043E-05	9.696441E-05	-6.771436E-05
7	C6	5.327482E-05	-1.626740E-04	-1.211905E-04
8	C7	-2.572767E-05	7.445352E-05	3.268646E-05
9	H3	2.945803E-05	-2.195525E-05	6.015338E-05
10	H4	1.924495E-05	-3.801340E-05	-1.645908E-05
11	H6	-9.022157E-06	1.760755E-05	-4.354284E-05
12	H7	3.457116E-05	-1.400594E-06	-1.432195E-05
13	C10	1.889606E-06	-9.010297E-05	-1.068424E-04
14	C8	-2.738016E-05	2.323841E-05	5.695785E-05
15	C17	1.357747E-05	-1.253223E-05	-1.044309E-04
16	N2	-5.643335E-05	-1.096662E-04	1.139320E-04
17	C9	-2.761392E-06	-1.579447E-05	-3.181960E-04
18	C16	1.261078E-04	3.550120E-04	-9.652122E-05
19	O1	6.101126E-05	-1.334813E-04	2.140386E-04
20	C11	-8.193691E-05	9.475484E-05	5.967980E-05
21	C12	3.496694E-05	-1.127337E-04	-1.453341E-04
22	C13	-1.600670E-04	-8.650379E-05	-1.794056E-04
23	C14	3.016052E-05	9.677616E-05	1.185685E-04
24	C15	1.619456E-04	8.884082E-05	1.504091E-04
25	H19	-3.645716E-05	1.322414E-05	-4.821011E-05
26	H20	5.076817E-05	-7.660128E-05	-5.050839E-05
27	H21	4.238381E-05	-3.476080E-06	7.993083E-06
28	H22	-5.727967E-05	8.436068E-05	1.129926E-05
29	H23	-1.118433E-05	3.047530E-05	-1.143174E-05
30	H27	-7.087251E-09	4.622415E-05	-7.413778E-06
31	H29	-5.302039E-07	-3.477520E-06	-8.306447E-06
32	H30	3.781358E-06	-3.265429E-06	-2.841010E-05
33	H15	5.481848E-07	-2.264069E-05	-5.782645E-06
34	H2	-3.173334E-05	-7.297815E-05	9.779004E-05
35	H5	1.289324E-05	-3.093760E-05	-6.087909E-05
36	H8	-2.357347E-05	-1.780480E-05	9.203421E-07
total		1.586710E-04	9.504341E-05	-3.880025E-04

```
 end of program der1b
```

```
  start of program geopt  13

  geometry optimization step 13
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format
  reading input hessian of dimension   108
   in five columns format


  energy change:          -3.7062E-05 *  (  5.0000E-05 )
  gradient maximum:        3.6955E-04 *  (  4.5000E-04 )
  gradient rms:            9.1746E-05 *  (  3.0000E-04 )
  step size:   0.00542  trust radius:   0.30000
  displacement maximum:    2.4588E-03 .  (  1.8000E-03 )
  displacement rms:        4.9083E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.3173E-06    geom step:   5.4214E-
03    full step:   5.4214E-03
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.4852E-06     y:    -2.1459E-04     z:     2.5391E-04

  new geometry:
                                angstroms
  atom            x                y                z
  H1       -0.2862833722     1.3318712197    -2.0567189923
  C1       -0.1809303267     1.7700071779    -1.0825824230
  C2        0.1205198605     2.9158186318     1.4060478219
  C3        0.2228741541     0.9735657038    -0.0245867913
  C4       -0.4430559476     3.1227927820    -0.9159086233
  C5       -0.2990027064     3.6886554031     0.3339084218
  C6        0.3972138629     1.5654874681     1.2344590411
  C7        0.5728168561    -0.5009512484    -0.1502123996
  H3       -0.7552325257     3.7176261849    -1.7554925941
  H4       -0.5077833713     4.7327653479     0.4875324188
  H6        0.2270454280     3.3737062088     2.3698120568
  H7        1.6613804333    -0.5476723650    -0.1673747349
  C10       0.0997435778    -1.2188480301    -1.4061059146
  C8        0.1555886063    -1.2395574787     1.1412004306
  C17      -1.3545750180    -1.3721271372     1.3932750753
  N2        0.8867295094     0.7956451202     2.3144567236
  C9        0.7836077976    -0.5707792817     2.3485491189
  C16       1.4395360943     1.4636187201     3.4846581109
  O1        1.1433115894    -1.2133552151     3.2959986320
  C11      -0.7037199330    -2.6659749470    -3.6670679695
  C12       0.9988269535    -2.0175696374    -2.1034479134
  C13      -1.2142912872    -1.1545979424    -1.8682416034
  C14      -1.6115320037    -1.8693248107    -2.9854114730
```

```
  C15       0.6045776246     -2.7370173862     -3.2219380212
  H19       2.0206757321     -2.0809454445     -1.7700125456
  H20      -1.9309775314     -0.5364735035     -1.3593970481
  H21      -2.6309237423     -1.8027277327     -3.3235608519
  H22       1.3211370524     -3.3479983340     -3.7424292123
  H23      -1.0136765307     -3.2208278063     -4.5349932315
  H27      -1.8545624388     -0.4089496519      1.3789730766
  H29      -1.8135638288     -2.0074385565      0.6473207082
  H30       0.5813486112     -2.2354361449      1.1221712883
  H15      -1.5159182988     -1.8256235508      2.3647628838
  H2        2.1046454804      2.2574820413      3.1695663181
  H5        1.9879642059      0.7373603124      4.0590449669
  H8        0.6577029716      1.8828427117      4.1103818663

  nuclear repulsion energy.......  1397.148047366 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  13   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    3.366E-04
  number of canonical orbitals.....          368
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H1     C1     C2     C3     C4     C5     C6
C7
  grid # 1       71     88     89     88     89     87     86
81
  grid # 2      115     96     95     97     97     97     93
90
  grid # 3      210    184    182    192    182    183    192
176
  grid # 4      208    327    326    340    327    327    328
312

  number of gridpoints:
     atom        H3     H4     H6     H7    C10     C8    C17
N2
  grid # 1       73     73     70     67     92     82     73
94
```

```
  grid # 2      118    118    112    106    100     90     80
104
  grid # 3      223    223    207    207    196    174    147
211
  grid # 4      224    223    206    204    341    314    286
390

  number of gridpoints:
     atom        C9    C16     O1    C11    C12    C13    C14
C15
  grid # 1       81     71    110     89     88     87     89
89
  grid # 2       91     79    122     97     95     95     95
97
  grid # 3      176    140    260    184    182    182    183
184
  grid # 4      293    272    456    328    326    325    326
328

  number of gridpoints:
     atom       H19    H20    H21    H22    H23    H27    H29
H30
  grid # 1       72     69     73     73     73     72     70
69
  grid # 2      112    111    118    118    118    110    109
109
  grid # 3      214    209    223    223    224    215    210
214
  grid # 4      213    205    223    223    224    212    207
208

  number of gridpoints:
     atom       H15     H2     H5     H8  total
  grid # 1       71     71     70     71   2861
  grid # 2      110    111    108    111   3724
  grid # 3      219    215    212    217   7175
  grid # 4      218    213    209    218   9910

  end of program grid


  start of program rwr
 recomputing RwR matrix  16    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density   DIIS
       r  t  s  t  d     total energy     change  change    error
```

```
etot   1  N  N  1  U  -783.03049309564           1.3E-05  2.5E-04
etot   2  Y  Y  4  M  -783.03050193703  8.8E-06  3.5E-06  7.7E-05
etot   3  Y  N  4  M  -783.03050255184  6.1E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion.....  1397.14804736617
   (E)  Total one-electron terms..... -3838.67138498744
   (I)  Total two-electron terms.....  1658.49283506943
   (L)  Electronic energy..... -2180.17854991801  (E+I)
   (N)  Total energy.............  -783.03050255184  (A+L)

 SCFE: SCF energy: HF    -783.03050255184 hartrees   iterations:
3


 HOMO energy:    -0.30120
 LUMO energy:     0.12991

  Orbital energies:
  -20.52431  -15.60127  -11.34396  -11.28549  -11.25550  -11.25112
  -11.24497  -11.24339  -11.24069  -11.23721  -11.23618  -11.23561
  -11.23487  -11.23415  -11.23371  -11.23343  -11.23334  -11.22834
  -11.21925   -1.39512   -1.26884   -1.16839   -1.14901   -1.10741
   -1.03260   -1.02091   -1.01901   -1.01558   -0.95805   -0.93990
   -0.85714   -0.84742   -0.83284   -0.82940   -0.78970   -0.74186
   -0.71154   -0.69811   -0.66965   -0.66203   -0.64791   -0.63525
   -0.63373   -0.61762   -0.61093   -0.60119   -0.60084   -0.58709
   -0.57713   -0.56654   -0.55175   -0.54758   -0.52445   -0.52138
   -0.51766   -0.51187   -0.50441   -0.49273   -0.48255   -0.47663
   -0.46694   -0.41960   -0.40855   -0.34091   -0.33681   -0.32829
   -0.30120    0.12991    0.13543    0.14005    0.14900    0.20693
    0.23321    0.24136    0.25592    0.26428    0.26847

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  16    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
```

1	H1	-1.987531E-05	-1.516714E-05	-1.903340E-05
2	C1	3.744530E-07	4.207960E-05	4.147687E-05
3	C2	1.578883E-05	-5.541063E-06	-4.642183E-05
4	C3	1.723961E-05	-5.782158E-06	7.209217E-06
5	C4	4.443375E-06	4.055476E-05	3.097308E-05
6	C5	-3.229671E-06	-2.178495E-05	-7.183730E-05
7	C6	-1.846592E-05	-2.394338E-05	-2.361599E-05
8	C7	-4.398903E-06	3.430284E-05	2.227726E-05
9	H3	-8.956332E-07	-1.258890E-05	2.183907E-05
10	H4	1.042585E-05	-1.593563E-05	-1.060012E-06
11	H6	2.751038E-05	6.990097E-06	1.027428E-05
12	H7	5.264690E-06	-7.826399E-06	-1.197869E-05
13	C10	-5.291733E-05	3.412756E-05	-2.622123E-05
14	C8	-6.317502E-06	-1.105236E-05	-8.245999E-06
15	C17	4.227870E-06	7.028878E-06	-1.887064E-05
16	N2	6.323661E-05	6.543782E-05	7.716588E-06
17	C9	4.207819E-06	-2.989634E-05	-1.904768E-05
18	C16	4.225031E-05	-3.369947E-05	-1.078110E-05
19	O1	1.564743E-05	-1.357047E-05	9.358162E-06
20	C11	5.515261E-05	-1.148810E-05	9.711405E-06
21	C12	4.311960E-06	-2.513094E-05	-5.856663E-05
22	C13	4.619916E-06	2.661507E-05	-2.454506E-05
23	C14	1.606979E-05	2.859720E-05	1.024806E-05
24	C15	-3.854745E-05	-1.033737E-05	-1.833781E-05
25	H19	1.706204E-06	-2.965837E-06	-7.619552E-06
26	H20	1.150856E-05	1.629952E-05	-2.895732E-05
27	H21	1.320055E-05	1.450251E-05	-1.157938E-05
28	H22	-9.853184E-06	-6.776160E-06	3.510858E-06
29	H23	1.440142E-06	-8.550372E-06	-9.347655E-06
30	H27	8.680040E-06	-1.384774E-05	-1.067727E-05
31	H29	2.153543E-05	2.004621E-05	-4.373160E-06
32	H30	-3.758161E-06	2.572625E-05	-1.379801E-05
33	H15	9.954203E-06	7.366788E-06	-3.337640E-05
34	H2	2.858579E-06	-2.214560E-06	-1.085833E-05
35	H5	-2.709828E-05	2.659405E-05	-5.259928E-05
36	H8	-4.805758E-06	-1.754611E-05	-8.034572E-06
total		1.714921E-04	1.006237E-04	-3.751894E-04

```
 end of program der1b


 start of program geopt  14

 geometry optimization step 14
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
 reading input hessian of dimension   108
  in five columns format
```

```
  energy change:           3.7250E-06 *  (  5.0000E-05 )
  gradient maximum:        2.0349E-04 *  (  4.5000E-04 )
  gradient rms:            4.6676E-05 #  (  3.0000E-04 )
  step size:   0.00392  trust radius:   0.30000
  displacement maximum:    1.4863E-03 *  (  1.8000E-03 )
  displacement rms:        3.5522E-04 *  (  1.2000E-03 )
  predicted energy change:    -5.3436E-07    geom step:   3.9236E-
03    full step:   3.9236E-03

  ***********************************************************
  **           Geometry optimization complete              **
  ***********************************************************

  center of mass moved by:
     x:     0.0000E+00     y:     0.0000E+00     z:     0.0000E+00

  final geometry:
                                 angstroms
  atom            x                 y                 z
  H1       -0.2862833722      1.3318712197     -2.0567189923
  C1       -0.1809303267      1.7700071779     -1.0825824230
  C2        0.1205198605      2.9158186318      1.4060478219
  C3        0.2228741541      0.9735657038     -0.0245867913
  C4       -0.4430559476      3.1227927820     -0.9159086233
  C5       -0.2990027064      3.6886554031      0.3339084218
  C6        0.3972138629      1.5654874681      1.2344590411
  C7        0.5728168561     -0.5009512484     -0.1502123996
  H3       -0.7552325257      3.7176261849     -1.7554925941
  H4       -0.5077833713      4.7327653479      0.4875324188
  H6        0.2270454280      3.3737062088      2.3698120568
  H7        1.6613804333     -0.5476723650     -0.1673747349
  C10       0.0997435778     -1.2188480301     -1.4061059146
  C8        0.1555886063     -1.2395574787      1.1412004306
  C17      -1.3545750180     -1.3721271372      1.3932750753
  N2        0.8867295094      0.7956451202      2.3144567236
  C9        0.7836077976     -0.5707792817      2.3485491189
  C16       1.4395360943      1.4636187201      3.4846581109
  O1        1.1433115894     -1.2133552151      3.2959986320
  C11      -0.7037199330     -2.6659749470     -3.6670679695
  C12       0.9988269535     -2.0175696374     -2.1034479134
  C13      -1.2142912872     -1.1545979424     -1.8682416034
  C14      -1.6115320037     -1.8693248107     -2.9854114730
  C15       0.6045776246     -2.7370173862     -3.2219380212
  H19       2.0206757321     -2.0809454445     -1.7700125456
  H20      -1.9309775314     -0.5364735035     -1.3593970481
  H21      -2.6309237423     -1.8027277327     -3.3235608519
  H22       1.3211370524     -3.3479983340     -3.7424292123
  H23      -1.0136765307     -3.2208278063     -4.5349932315
  H27      -1.8545624388     -0.4089496519      1.3789730766
  H29      -1.8135638288     -2.0074385565      0.6473207082
```

```
 H30       0.5813486112     -2.2354361449      1.1221712883
 H15      -1.5159182988     -1.8256235508      2.3647628838
 H2        2.1046454804      2.2574820413      3.1695663181
 H5        1.9879642059      0.7373603124      4.0590449669
 H8        0.6577029716      1.8828427117      4.1103818663

 nuclear repulsion energy.......  1397.148047366 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  14   /
------------------------------------------------

 end of program geopt


 start of program post
 Writing a SPARTAN archive file
 end of program post

Total cpu seconds     user:     965.859   user+sys:     965.859
```

Summary calculation on *trans* (**9**) and *cis* (**10**) derivatives

Sample	stereo	HF	ΔG	% rel	weighted HF	ΔG	% rel
Trans 1	(eq-eq)	-491330.559	0.654	75	491330.390	0.593	73
Trans 2	(ax-ax)	-491329.905		25			
Cis 1	(Ph eq_met ax)	-491328.149	1.732	5	491329.797		27
Cis 2	(Ph ax_met eq)	-491329.881		95			