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Higher-Order Cyclization Reactions of Alkenyl Fischer Carbene Complexes: A New Selective All-Carbon [8 + 2] Cyclization with 8-Methoxyheptafulvene and Computational Mechanistic Analysis

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Supporting Information

1. NMR Spectra..... S2

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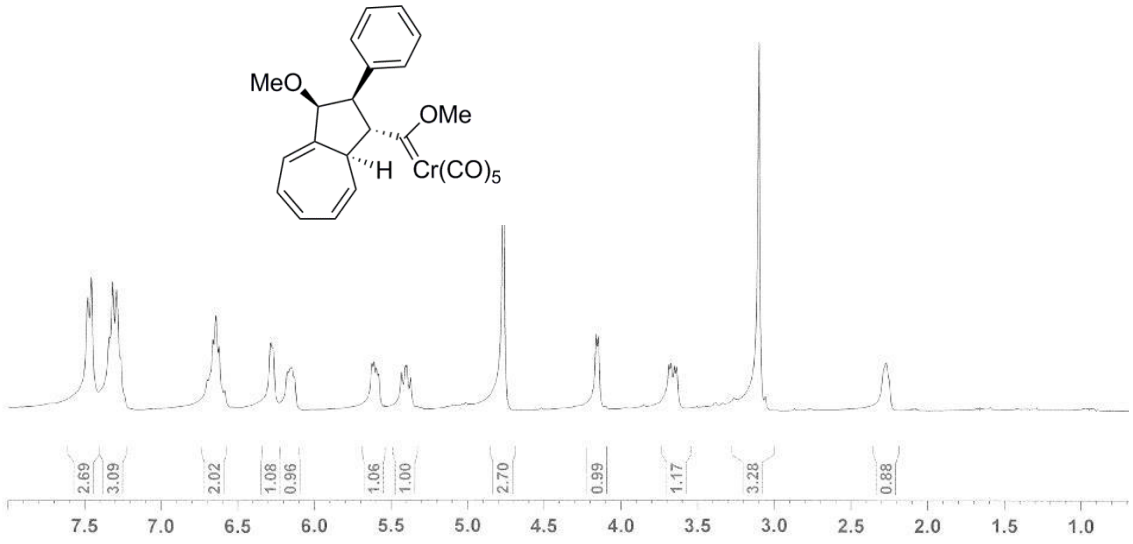
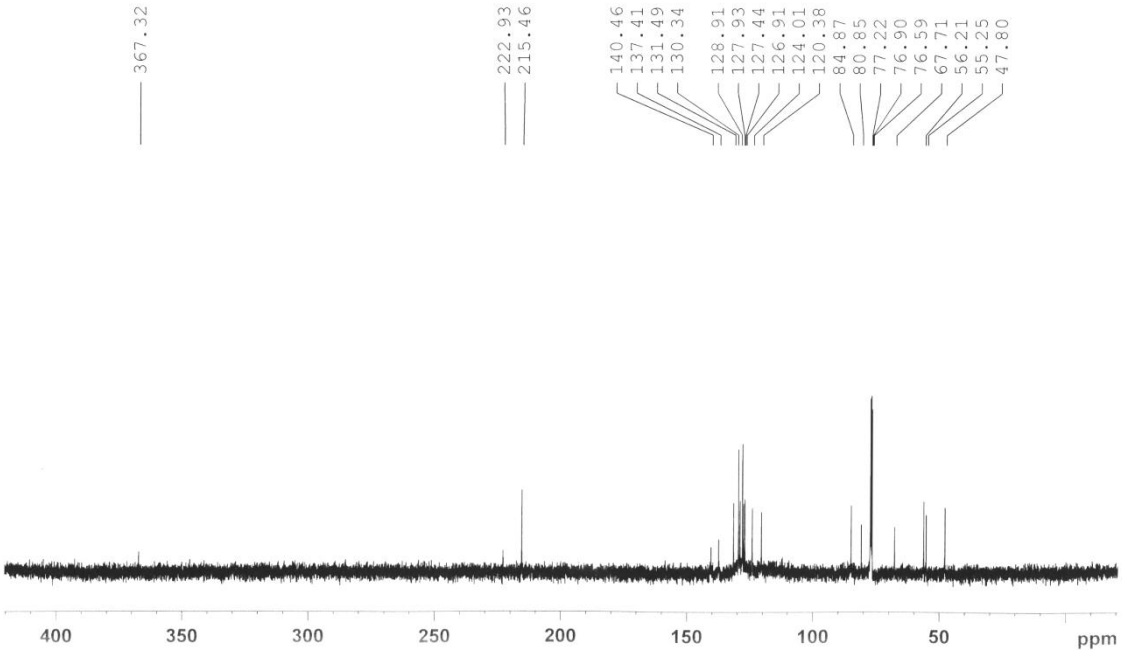
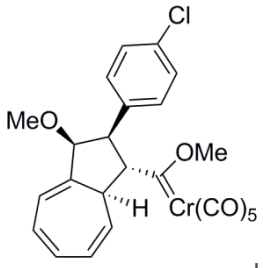
1. NMR Spectra

3a

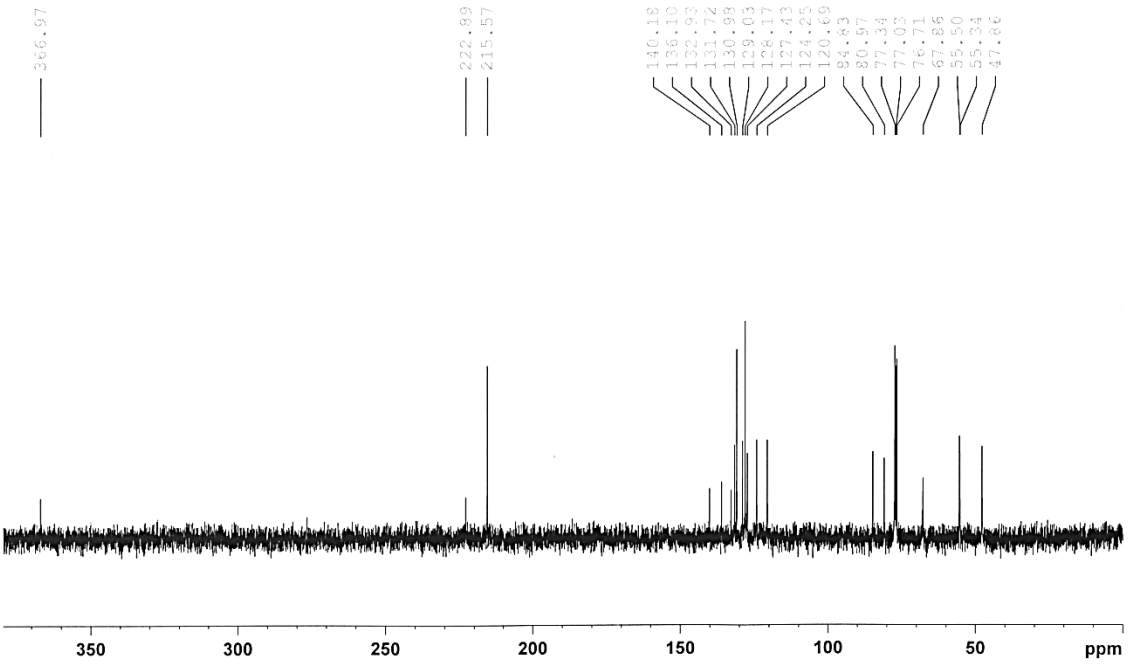




3c


Cl
MeO
OMe
H
Cr(CO)5

7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0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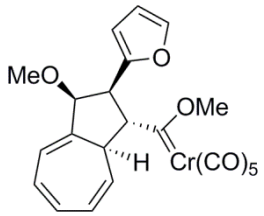
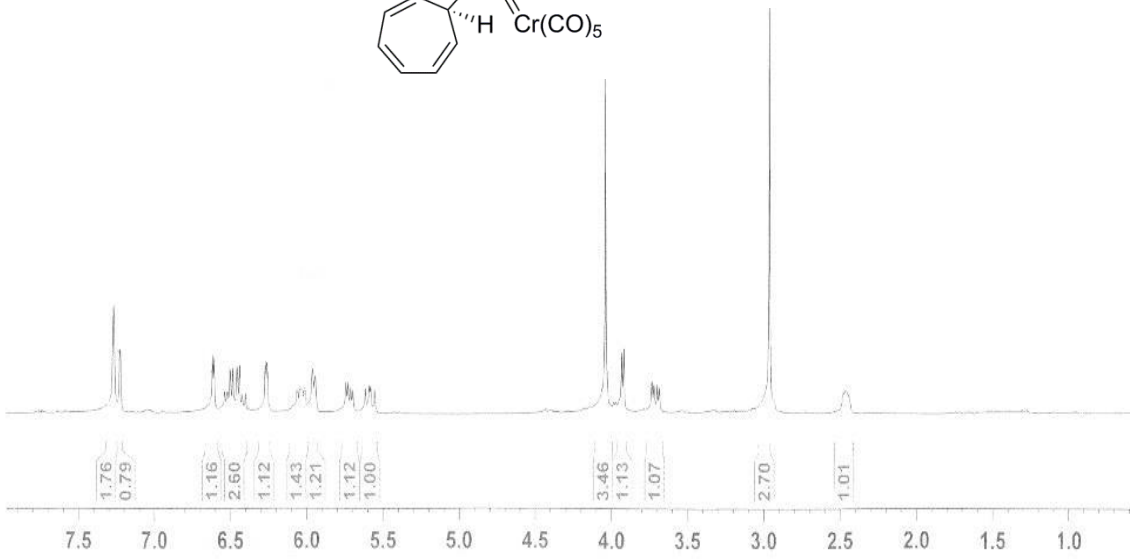
222.99
215.57
140.18
136.10
132.93
131.72
130.99
129.03
128.17
127.43
124.25
120.69
84.83
80.97
77.34
77.03
76.71
67.86
55.50
55.34
47.86
350
300
250
200
150
100
50
ppm

3e


MeO
O
OMe
H
Cr(CO)5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1.43
1.21
1.12
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3.46
1.13
1.07
2.70
1.01
7.5
7.0
6.5
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5.0
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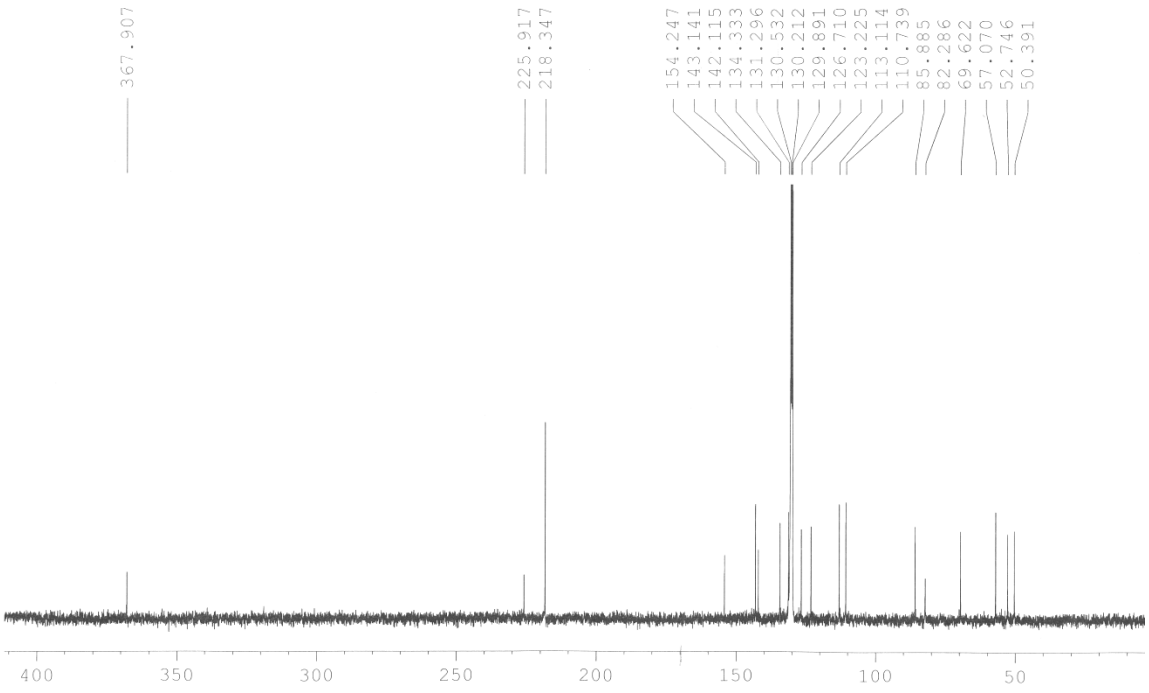
4.0
3.5
3.0
2.5
2.0
1.5
1.0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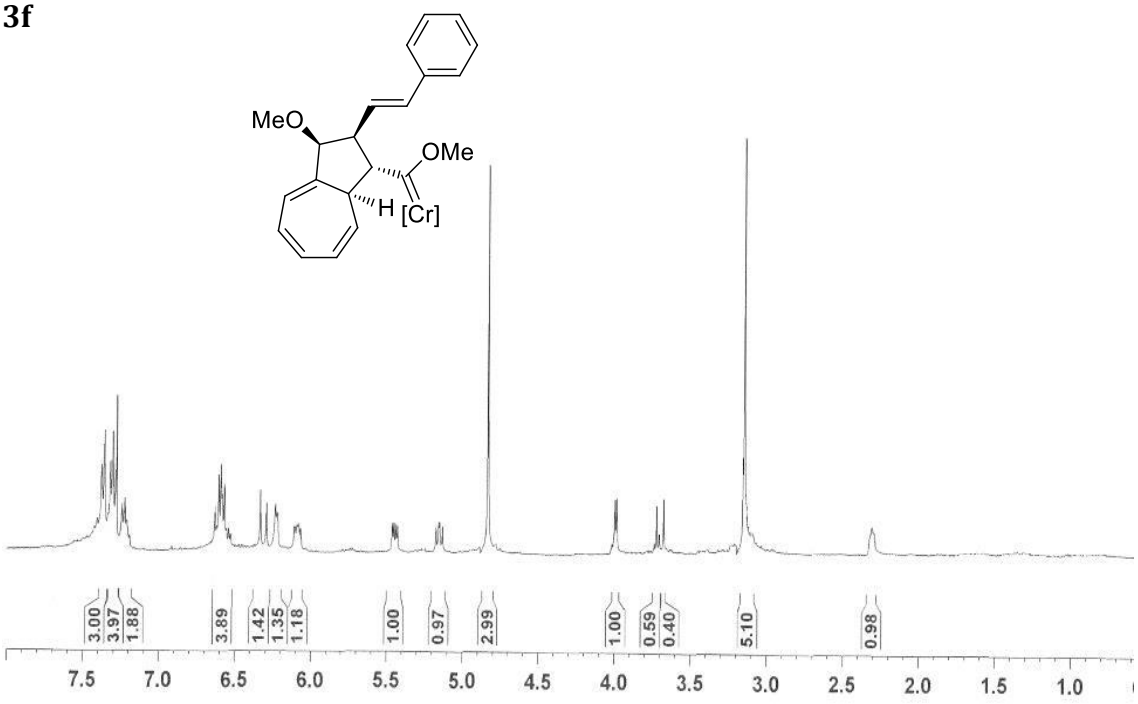
225.917
218.347
154.247
143.141
142.115
134.333
131.296
130.532
130.212
129.891
126.710
123.225
113.114
110.739
85.885
82.286
69.622
57.070
52.746
50.391
400
350
300
250
200
150
100
50

3f


MeO
OMe
H
[Cr]
3.00
3.97
1.88
3.89
1.42
1.35
1.18
1.00
0.97
2.99
1.00
0.59
0.40
5.10
0.98
7.5
7.0
6.5
6.0
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4.5
4.0
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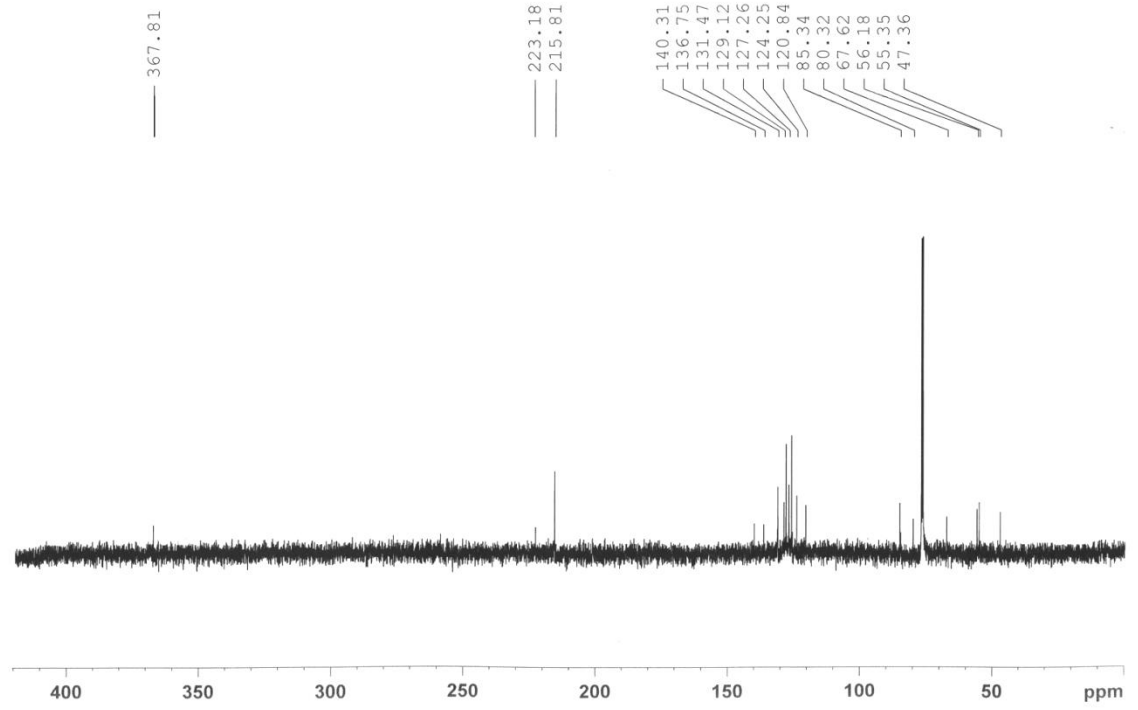
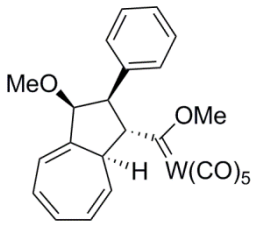
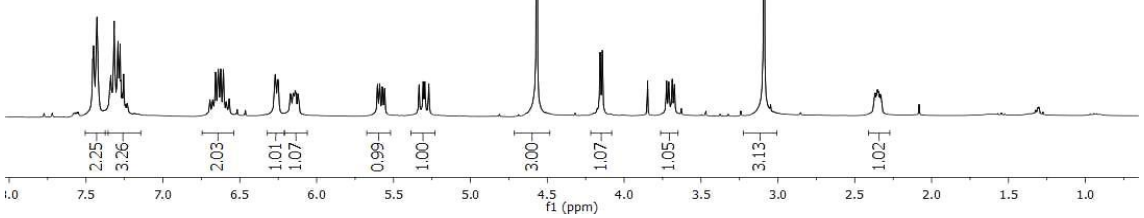
3.0
2.5
2.0
1.5
1.0

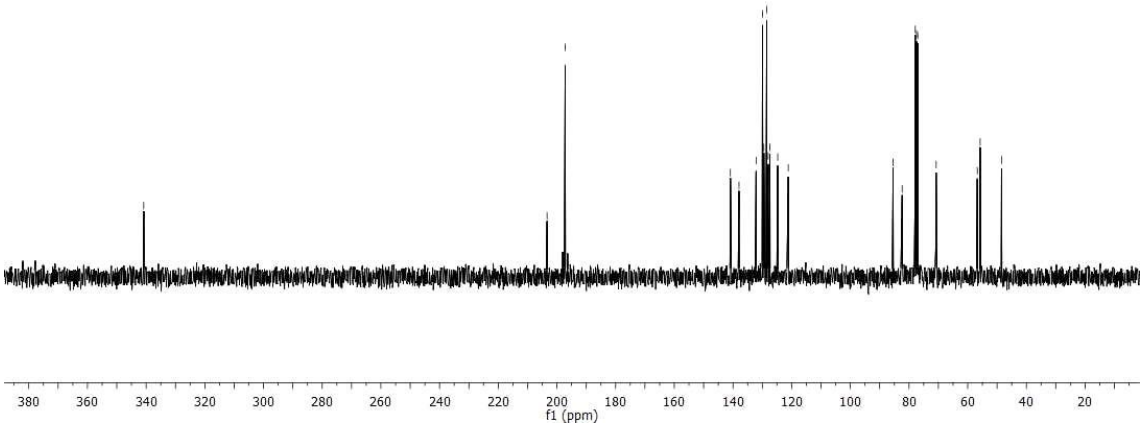

367.81
223.18
215.81
140.31
136.75
131.47
129.12
127.26
124.25
120.84
85.34
80.32
67.62
56.18
55.35
47.36
400
350
300
250
200
150
100
50
ppm

3g

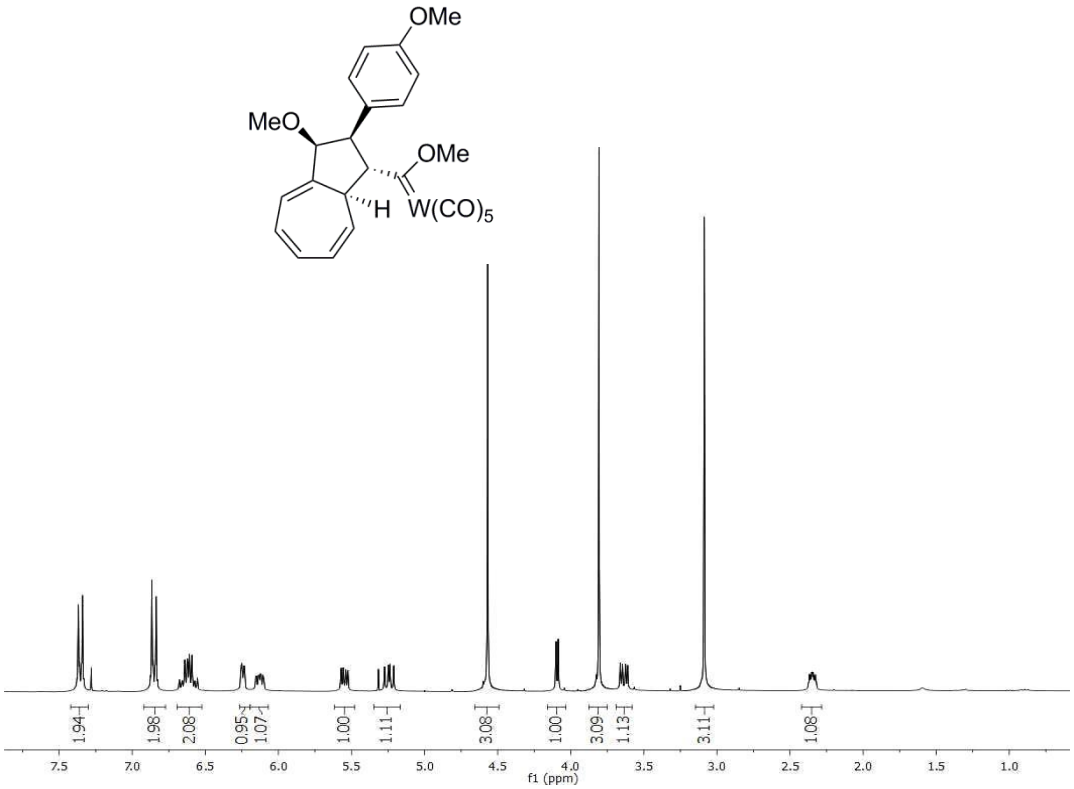

MeO
OMe
H
W(CO)5

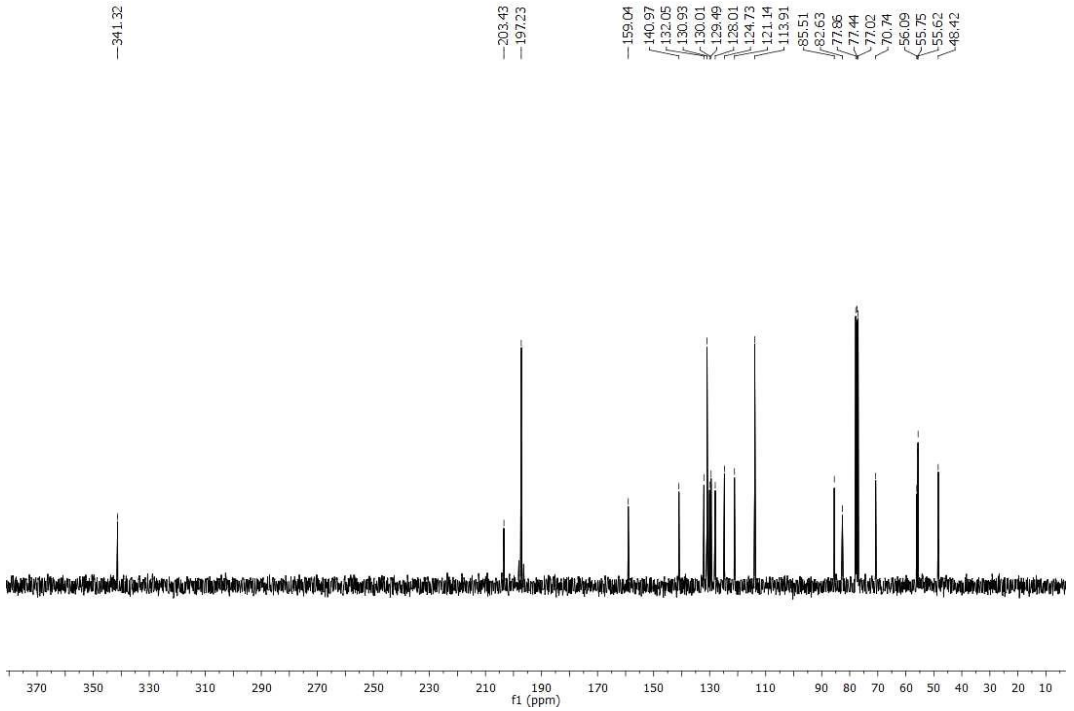

2.25
3.26
2.03
1.01
1.07
0.99
1.00
3.00
1.07
1.05
3.13
1.02
f1 (ppm)


340.81
203.36
197.20
140.87
137.95
132.13
129.93
129.48
128.49
128.01
127.40
124.75
121.15
85.43
82.34
77.87
77.45
77.03
70.75
56.73
55.76
48.47


f1 (ppm)

3h


OMe
MeO
OMe
H
W(CO)5
1.94
1.98
2.08
0.95
1.07
1.00
1.11
3.08
1.00
3.09
1.13
3.11
1.08
f1 (ppm)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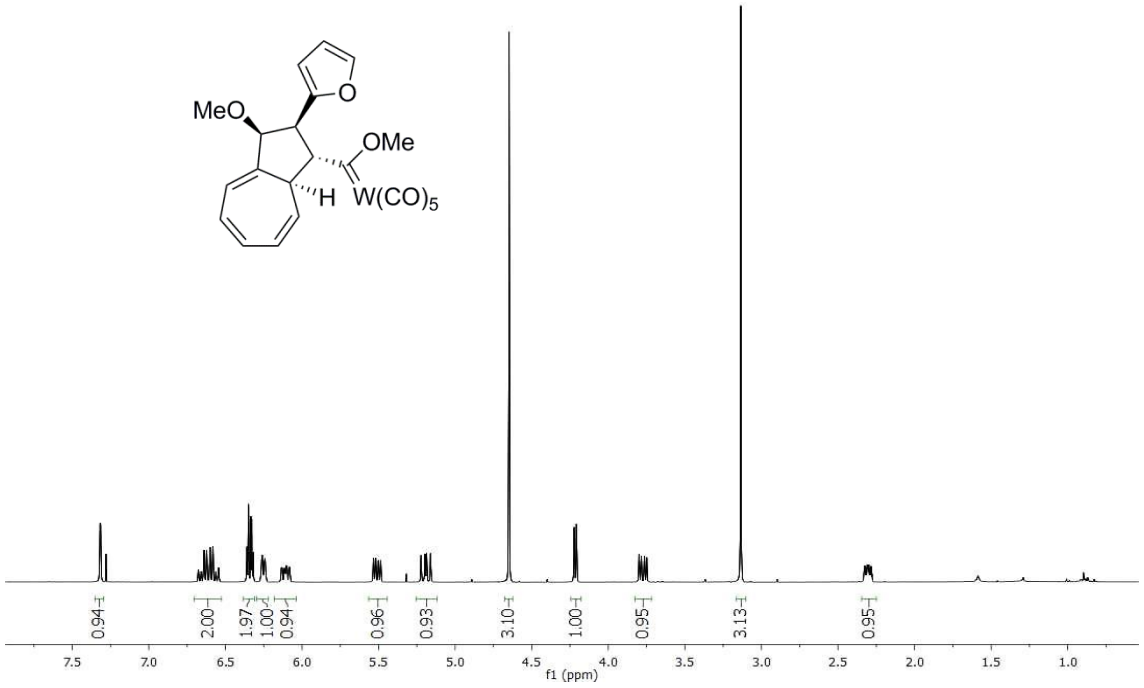
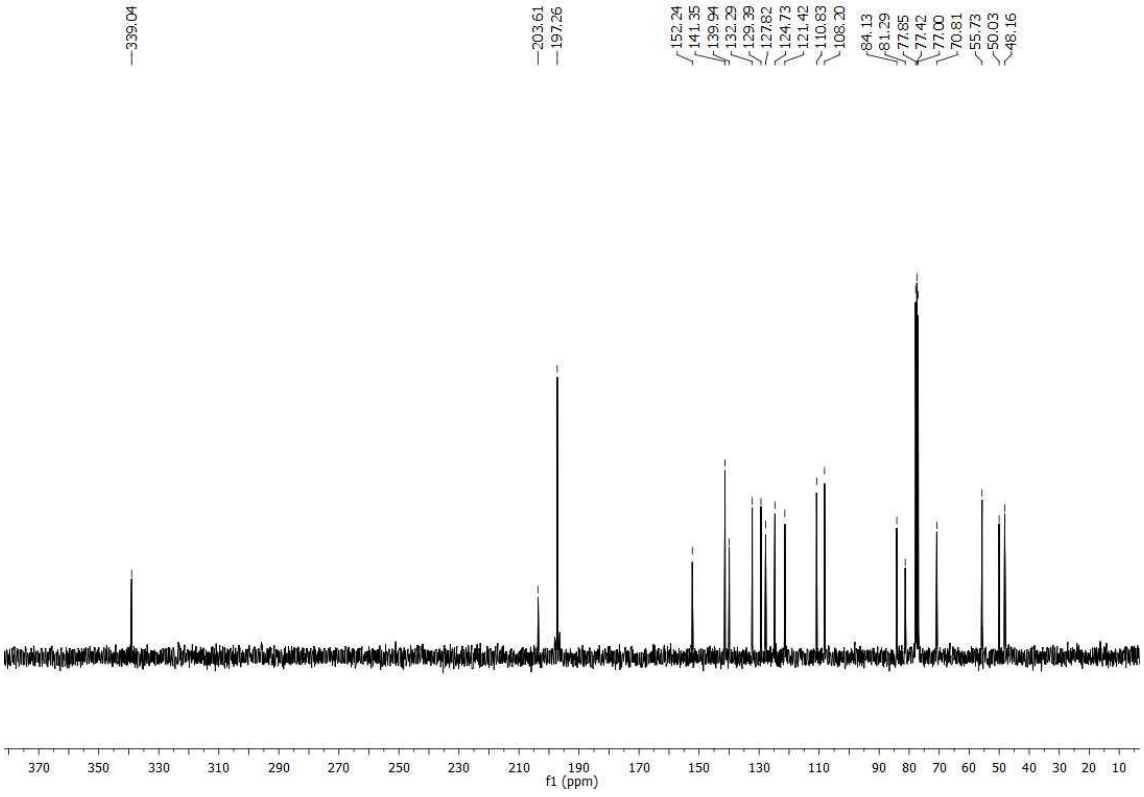
159.04
140.97
132.05
130.93
130.01
129.49
128.01
124.73
121.14
113.91
85.51
82.63
77.86
77.44
77.02
70.74
56.09
55.75
55.62
48.42
f1 (ppm)

3i


MeO
O
OMe
H
W(CO)5
0.94
2.00
1.97
1.00
0.94
0.96
0.93
3.10
1.00
0.95
3.13
0.95
f1 (ppm)


339.04
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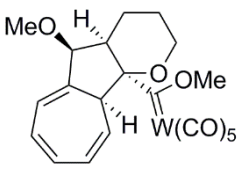
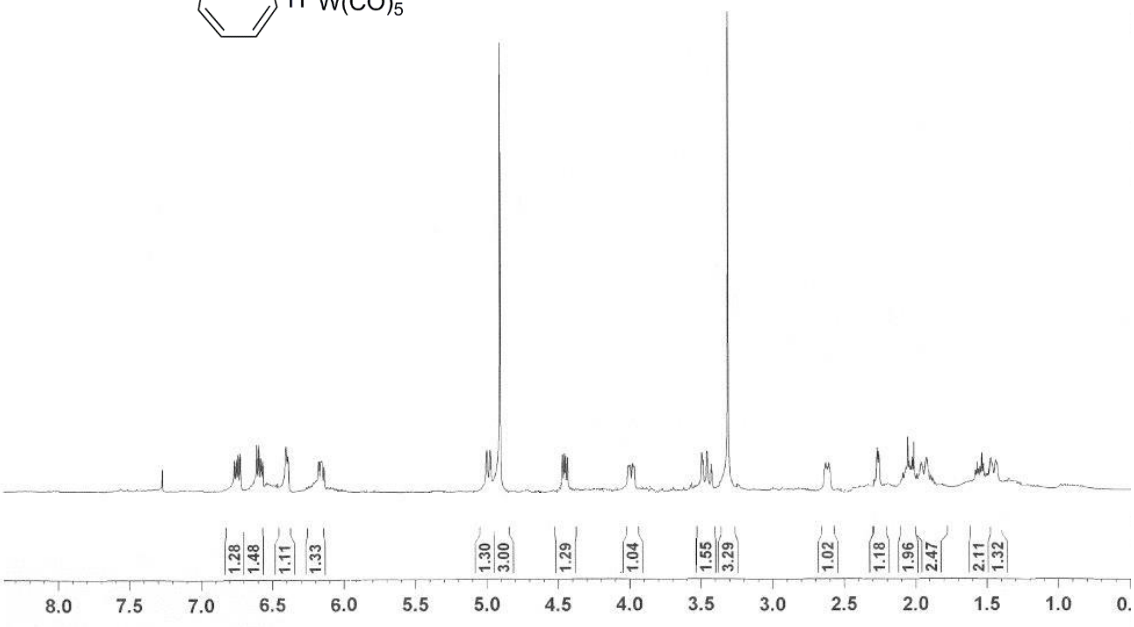
197.26
152.24
141.35
139.94
132.29
129.39
127.82
124.73
121.42
110.83
108.20
84.13
81.29
77.85
77.42
77.00
70.81
55.73
50.03
48.16
f1 (ppm)

3j


MeO
H
O
OMe
H
W(CO)5


1.28
1.48
1.11
1.33
1.30
3.00
1.29
1.04
1.55
3.29
1.02
1.18
1.96
2.47
2.11
1.32
8.0
7.5
7.0
6.5
6.0
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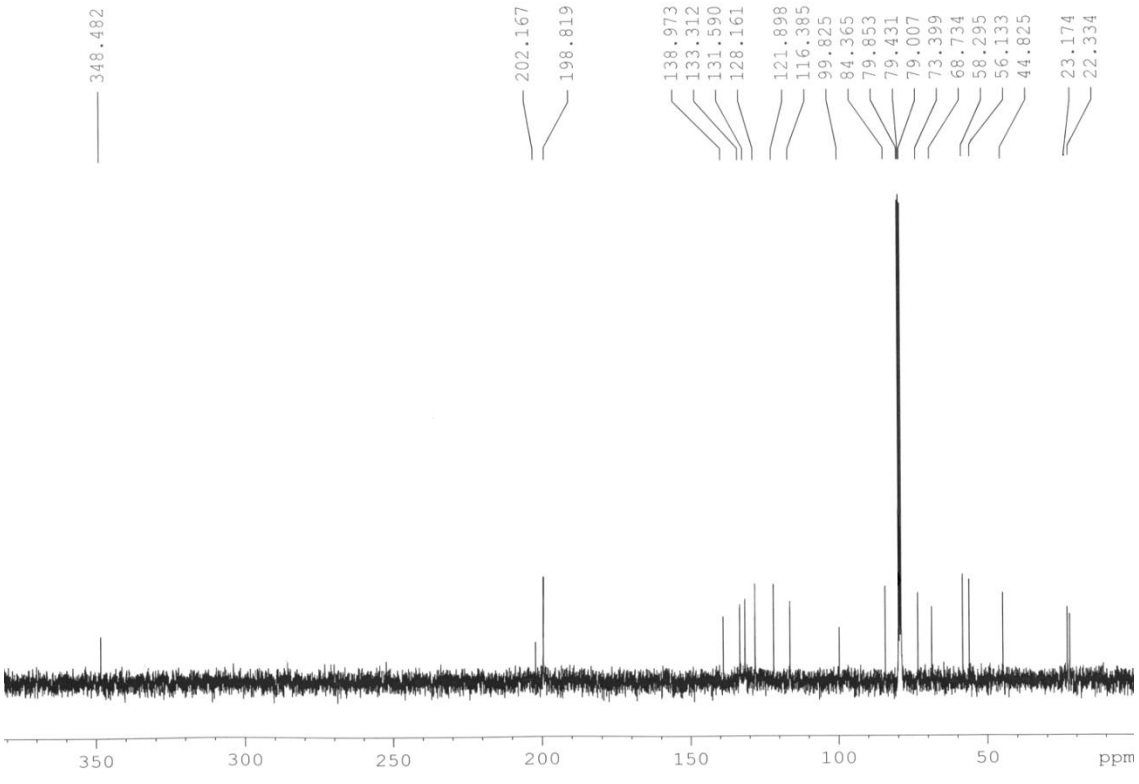
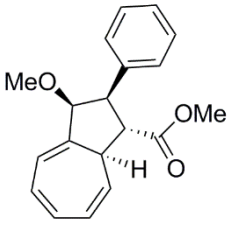
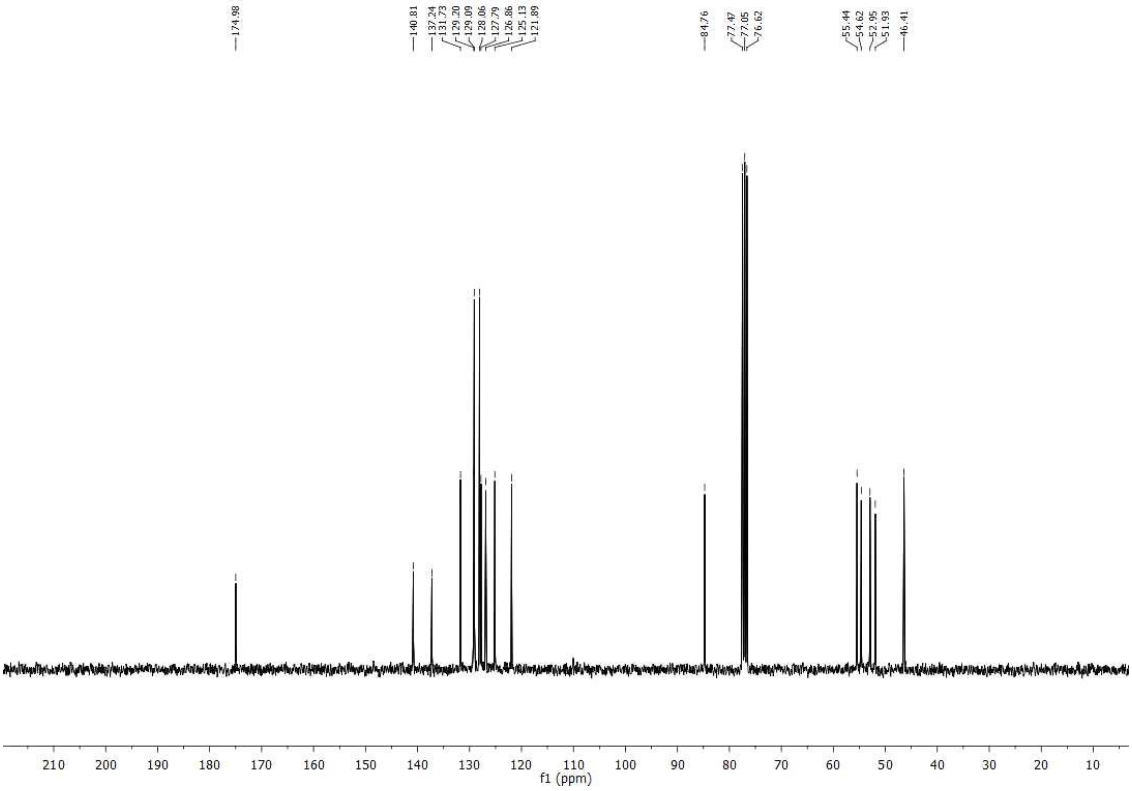
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0


348.482
202.167
198.819
138.973
133.312
131.590
128.161
121.898
116.385
99.825
84.365
79.853
79.431
79.007
73.399
68.734
58.295
56.133
44.825
23.174
22.334
350
300
250
200
150
100
50
ppm

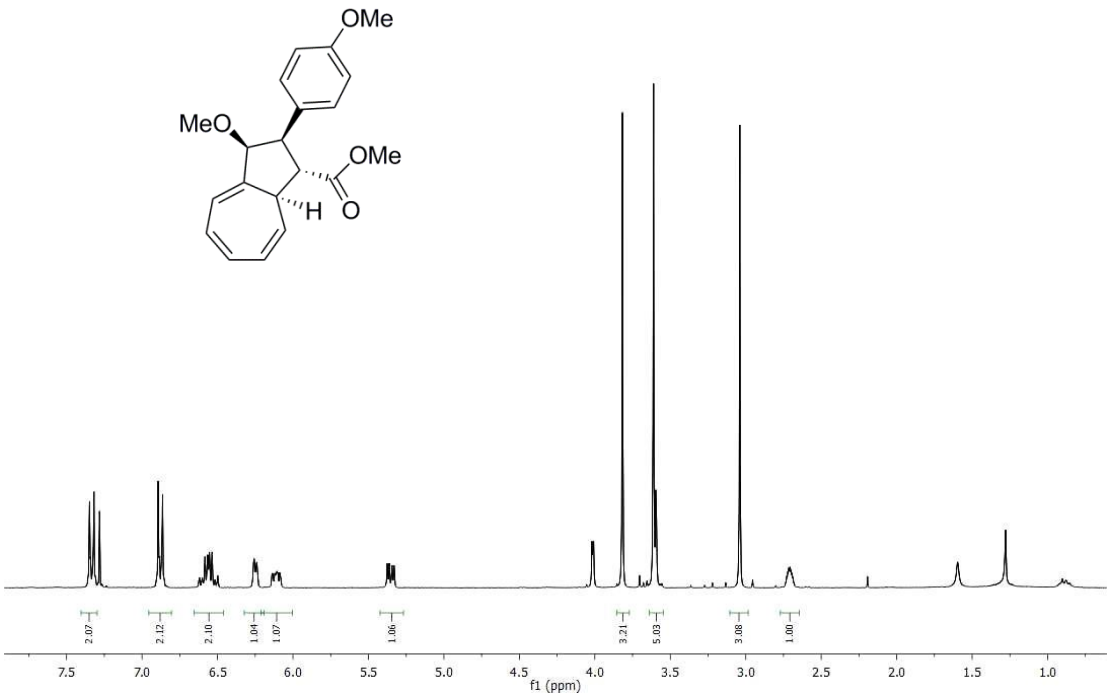
4a

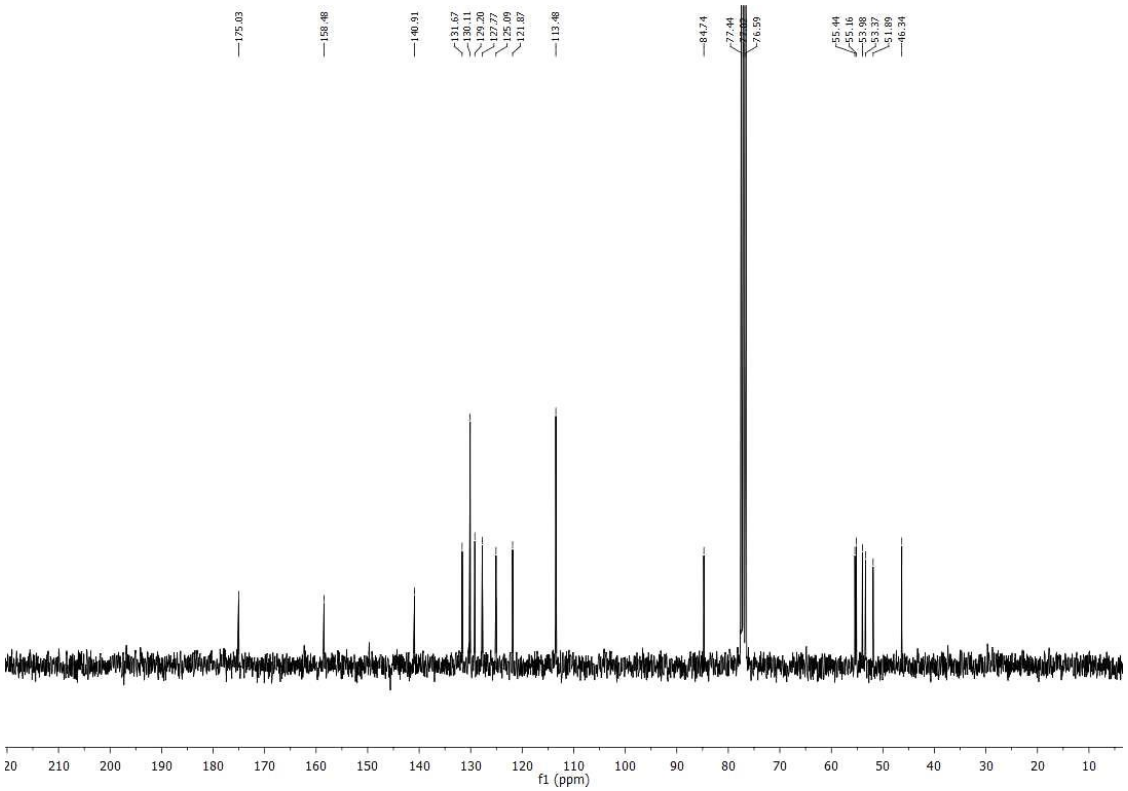

MeO
OMe
O
H

5.39
2.00
0.98
0.96
1.01
1.05
1.83
2.91
3.01
0.94
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)


174.98
140.81
137.24
133.23
129.20
129.09
128.06
127.79
126.86
125.13
121.89
84.76
77.47
77.05
76.62
55.44
54.62
52.95
51.93
46.41
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

4b


OMe
MeO
OMe
H
O
2.07
2.12
2.10
1.04
1.07
1.06
3.21
5.03
3.08
1.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)


175.03
158.48
140.91
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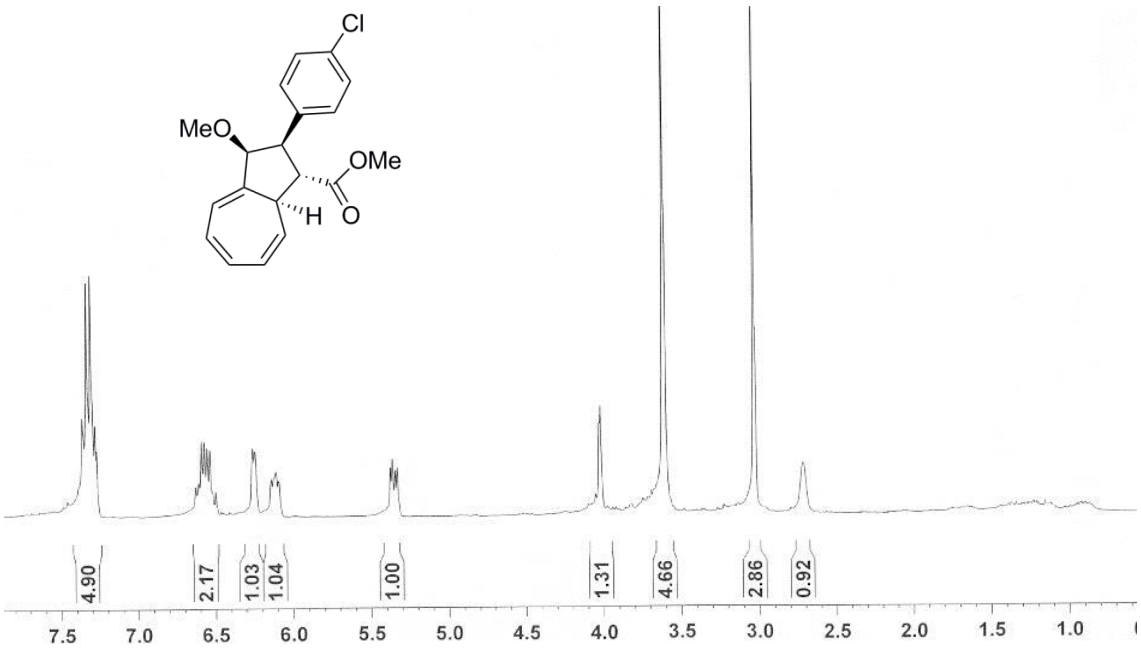
130.11
129.20
127.77
125.09
121.87
113.48
84.74
77.44
76.59
55.44
55.16
53.98
53.37
51.89
46.34
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

4c


Cl
MeO
OMe
H
O
4.90
2.17
1.03
1.04
1.00
1.31
4.66
2.86
0.92
7.5
7.0
6.5
6.0
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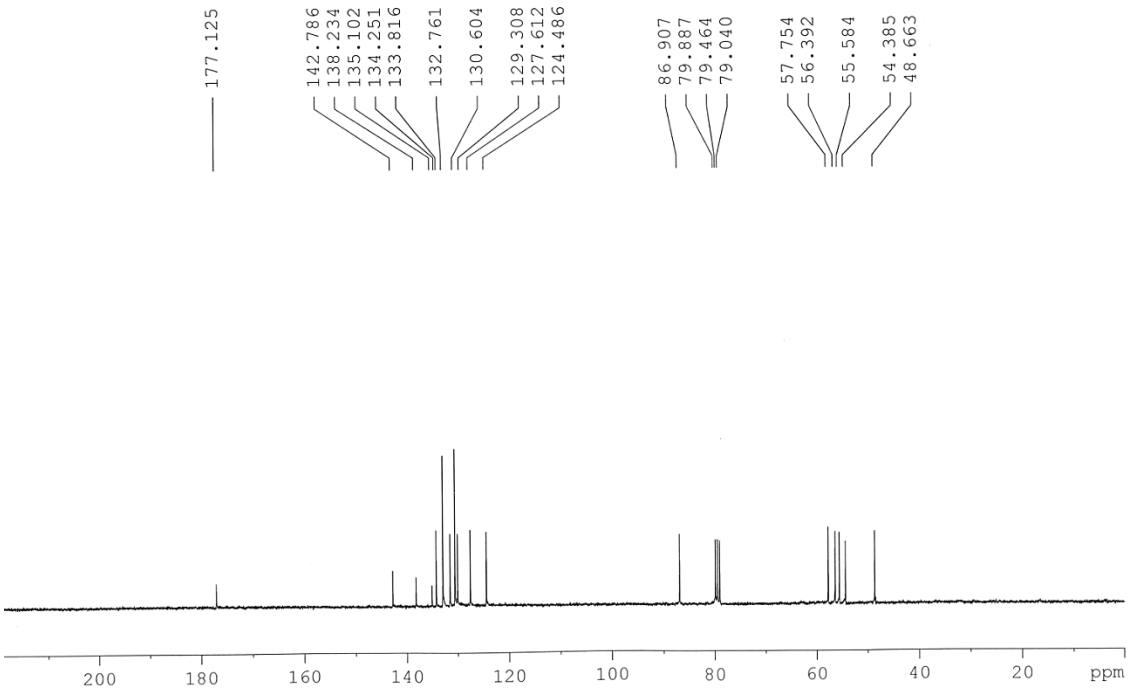
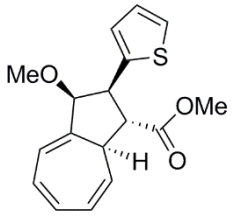
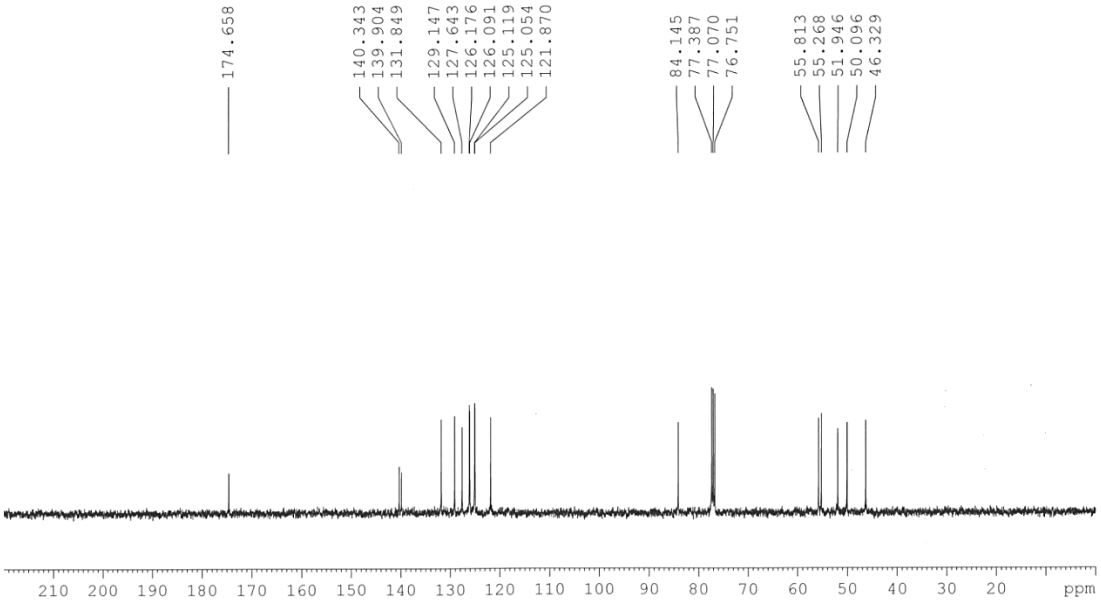
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0


177.125
142.786
138.234
135.102
134.251
133.816
132.761
130.604
129.308
127.612
124.486
86.907
79.887
79.464
79.040
57.754
56.392
55.584
54.385
48.663
200
180
160
140
120
100
80
60
40
20
ppm

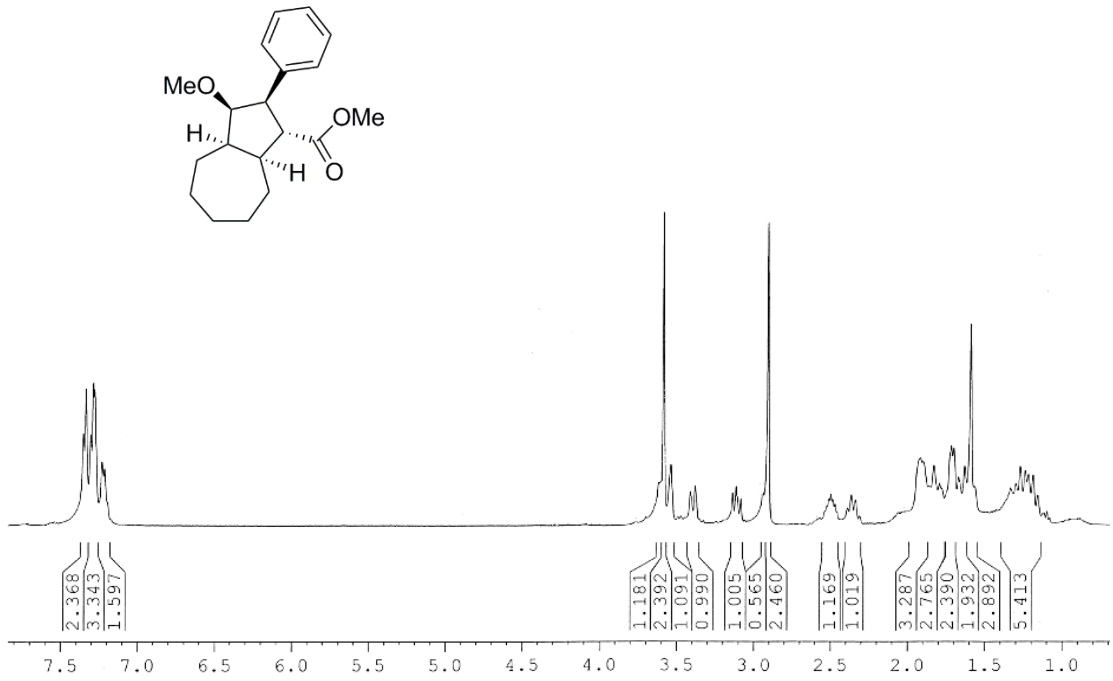
4d

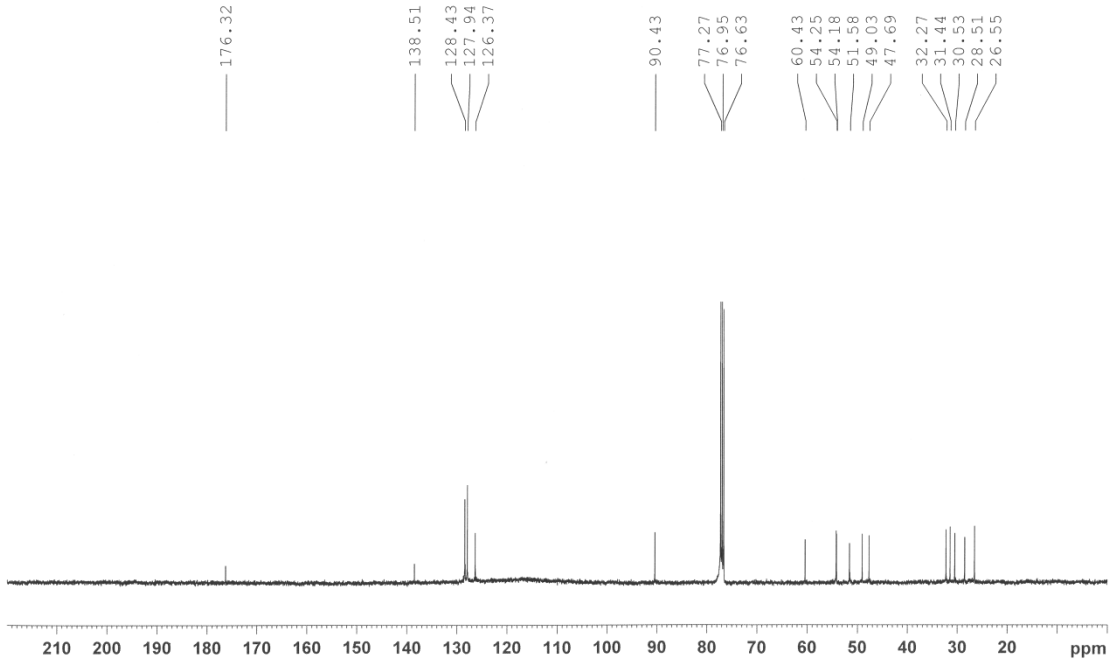

MeO
S
OMe
H
O

0.94
1.02
1.02
2.35
1.17
1.08
1.00
1.16
1.17
2.91
1.10
3.23
1.03
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0


174.658
140.343
139.904
131.849
129.147
127.643
126.176
126.091
125.119
125.054
121.870
84.145
77.387
77.070
76.751
55.813
55.268
51.946
50.096
46.329
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

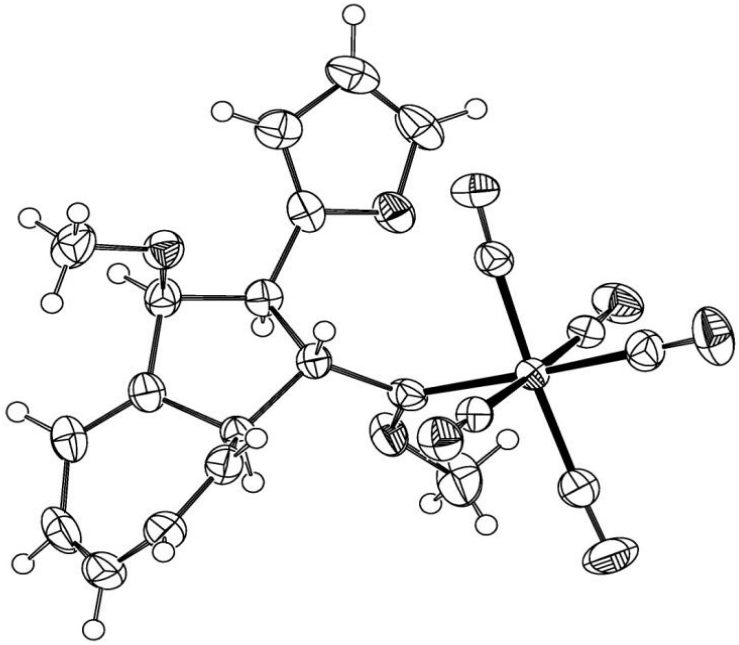
5


MeO
OMe
H
H
O
2.368
3.343
1.597
1.181
2.392
1.091
0.990
1.005
0.565
2.460
1.169
1.019
3.287
2.765
2.390
1.932
2.892
5.413
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0


176.32
138.51
128.43
127.94
126.37
90.43
77.27
76.95
76.63
60.43
54.25
54.18
51.58
49.03
47.69
32.27
31.44
30.53
28.51
26.55
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

2. X-Ray Data

Cristal structure data for $C_{22}H_{18}CrO_8$ *(3e)*



50% probability level

M_r = 462.36; T = 293 (2) K; λ = 0.71073 Å; **Crystal system:** Orthorhombic; **Space group:** *Pbca*.

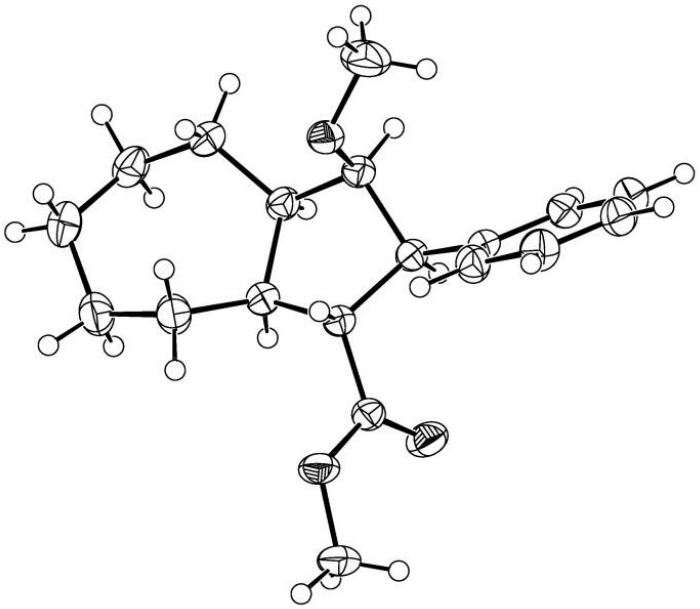
Unit cell dimensions: a = 12.5048 (2), b = 16.5248 (3), c = 21.1589 (4) Å, $\alpha = \beta = \gamma$ = 90.00º. **Volumen =** 4372.26 (13) $Å^3$; Z = 8**, Calculated density =** 1.405 Mgm^{-3}

F(000) = 1904; **Crystal size:** 0.5 x 0.25 x 0.1 mm.

θ**range data collection =** 1.018-25.082; **Index ranges:** $0 \leq h \leq 15$, $0 \leq k \leq 19$, $0 \leq l \leq 25$; **Reflections collected/unique =** 21876/3946 [R_{int} = 0.04]; **Completeness to** 2θ **=** 25.24 (99.9%); **Absortion correction:** Semiempirical from equivalents; **Max. and min. transmission =** 1.047 and 0.568; **Refinement method:** full matrix least-squares on F^2; **Data /restraints / parameters =** 3946 / 0 / 280; **Goodness-of-fit on** F^2 **=** 1.156; **Final** R **indices [**$I > 2\sigma(I)$**]:** R_1 = 0.0514, wR_2 = 0.1449; R **indices (all data):** R_1 = 0.0701, wR_2 = 0.1776; **Largest difference peak and hole =** 1.255 and -0.595 $eÅ^{-3}$.

Deposit number: CCDC 1026105

Cristal structure data for $C_{19}H_{26}O_3$ *(5)*



50% probability level

M_r = 302.40; T = 150 (2) K; λ = 1.54184 Å; **Crystal system:** Triclinic; **Space group:** *P-1*.

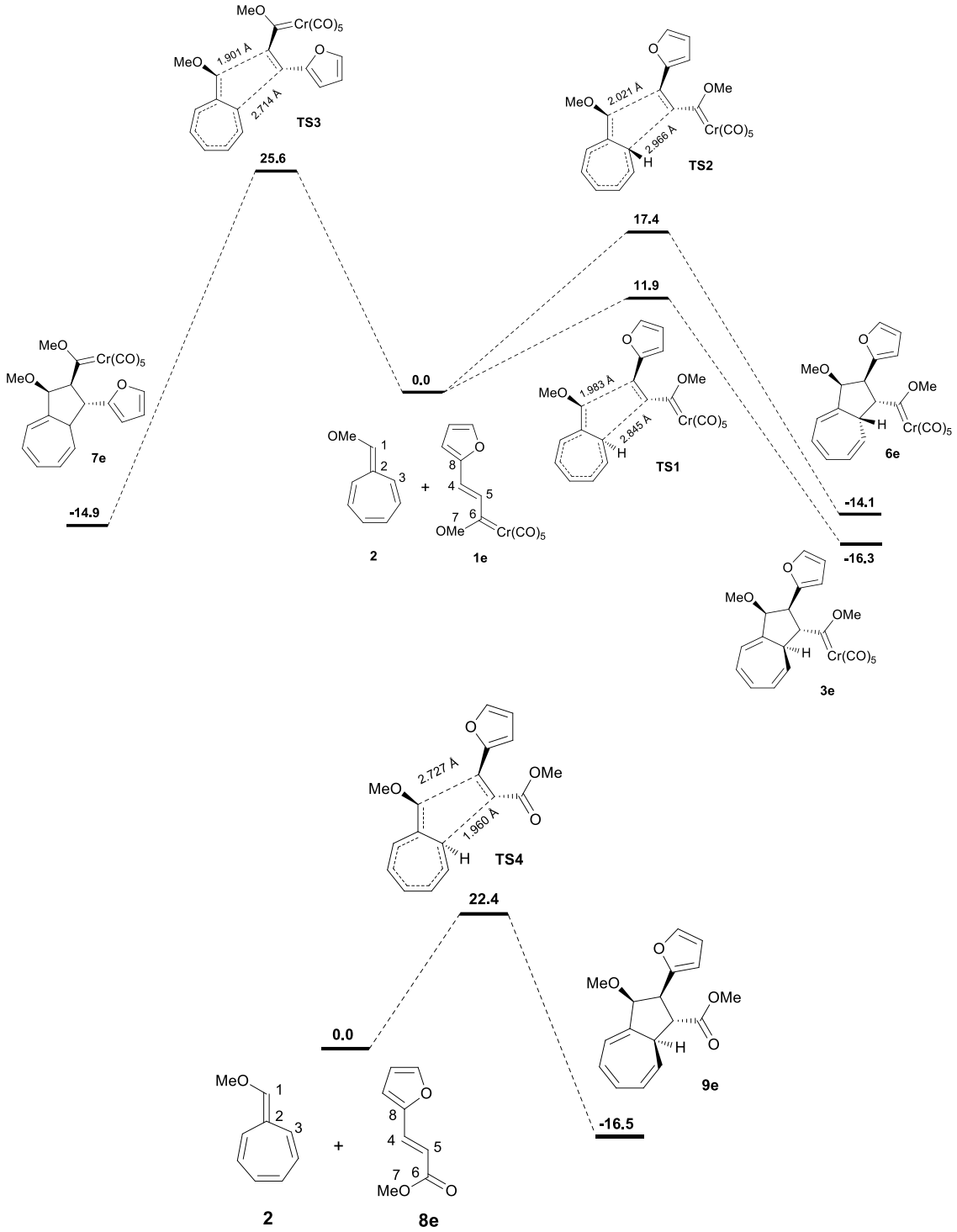
Unit cell dimensions: a = 8.9457 (4), b = 9.2864 (5), c = 11.7075 (5) Å, α = 100.602 (4), β = 98.957 (4)º, γ = 115.369 (5). **Volumen =** 833.13 (7) Å^3; Z = 2**, Calculated density =** 1.205 Mgm^{-3}

F(000) = 328; **Crystal size:** 0.3 x 0.16 x 0.15 mm.

θ**range data collection =** 3.974-77.555º; **Index ranges:** -10≤h≤10, -10≤k≤11, -11≤l≤14; **Reflections collected/unique =** 7828/3068 [R_{int} = 0.0112]; **Completeness to** 2θ **=** 70.00(94.5%); **Absortion correction:** Semiempirical from equivalents; **Max. and min. transmission =** 1.0000 and 0.4920; **Refinement method:** full matrix least-squares on F^2; **Data /restraints / parameters =** 3068/0/201; **Goodness-of-fit on** F^2 **=** 1.073; **Final** R **indices [**$I>2\sigma(I)$**]:** R_1 = 0.0402, wR_2 = 0.1036; R **indices (all data):** R_1 = R_1 = 0.0422, wR_2 = 0.1104; **Largest difference peak and hole =** 0.254 and -0.189 eÅ^{-3}.

Deposit number: CCDC 1026104

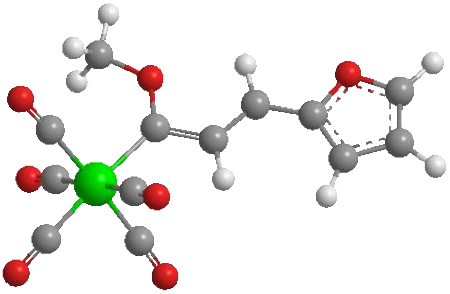
3. Cartesian Coordinates and Free Energies for the Calculated Geometries (PCM-B3PW91-D3/cc-pVDZ//B3PW91/cc-pVDZ level)



Model compound 1e;

E: -2070,820016 u.a.

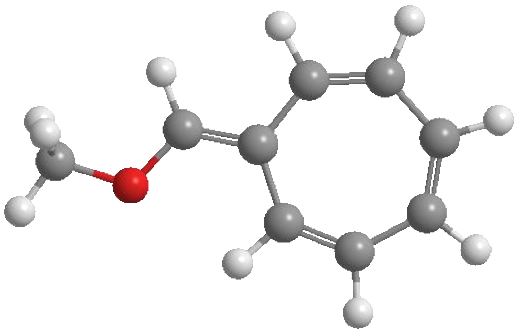
Cr	-1.418250	-1.013888	-0.107642
O	0.777942	-0.341317	1.957820
O	-2.213267	1.755471	-1.086100
O	4.078323	2.821626	0.505915
O	-3.255784	-0.615803	2.282559
O	0.224635	-1.489387	-2.624306
O	-0.808389	-3.869807	0.740838
O	-3.822653	-2.121482	-1.584317
C	2.995428	2.334865	-0.181484
C	2.180310	1.392974	0.515839
C	2.965071	2.907694	-1.438713
C	-2.908586	-1.701810	-1.019987
C	4.716448	3.685081	-0.306177
C	0.245311	-0.171305	0.752743
C	1.063673	0.789640	0.020734
C	4.080154	3.780896	-1.516067
C	-2.522465	-0.760000	1.403933
C	0.216644	-1.221664	2.926428
C	-1.009659	-2.771689	0.450756
C	-1.896624	0.714609	-0.708972
C	-0.382399	-1.300610	-1.664223
H	2.505485	1.155714	1.531711
H	2.224323	2.717847	-2.210987
H	5.604419	4.156544	0.104831
H	0.736016	1.023739	-0.992799
H	4.378825	4.402731	-2.355744
H	0.871312	-1.144179	3.803358
H	0.211821	-2.255811	2.559048
H	-0.800490	-0.909761	3.195854



Model compound 2;

E: -423,878737 u.a.

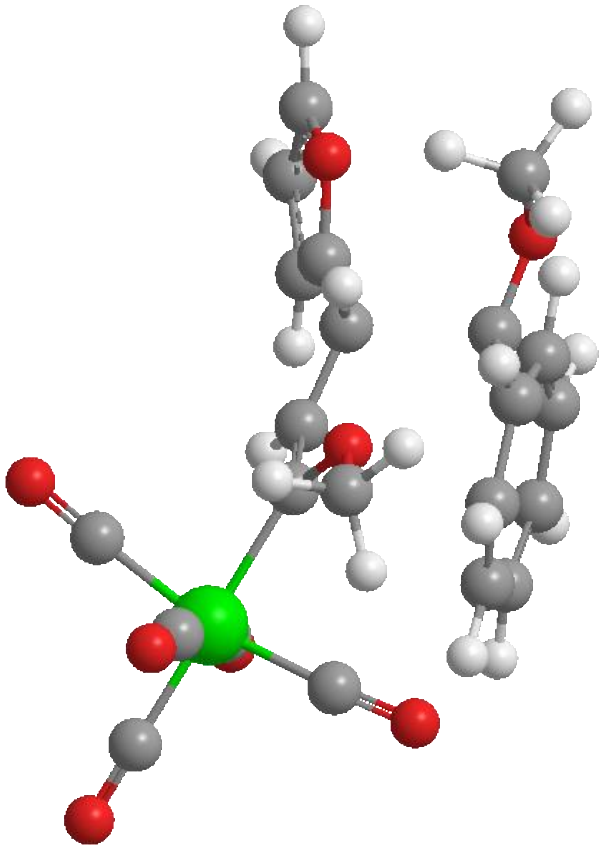
O	1.668431	0.928019	1.751443
C	0.623214	0.077102	1.589772
C	0.019054	-0.104600	0.382008
C	-1.078636	-1.061472	0.322666
C	0.067074	0.643025	-2.061361
C	-1.810801	-1.042144	-2.107820
C	-0.985289	-0.138227	-2.687401
C	0.490101	0.657506	-0.775209
C	2.090718	1.110357	3.087601
C	-1.850821	-1.457871	-0.718056
H	0.297231	-0.469596	2.481564
H	-1.308138	-1.532250	1.285903
H	0.594835	1.320746	-2.739817
H	-2.545705	-1.527043	-2.757759
H	-1.117826	0.036219	-3.759435
H	1.311783	1.339439	-0.542362
H	2.952853	1.788957	3.058380
H	2.402196	0.154770	3.547197
H	1.295602	1.564642	3.705854
H	-2.617957	-2.202092	-0.484267



Model compound TS1;

E: -2494,679755 u.a. (407i)

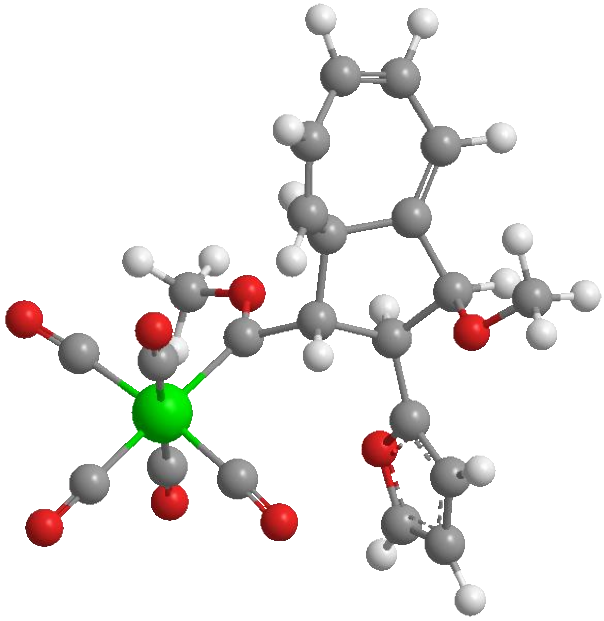
Cr	2.793064	-0.286152	0.144480
O	0.315932	-0.858420	2.022362
O	-3.860475	-0.113769	1.428361
O	2.475258	-2.903915	-1.378361
O	-3.545511	-2.310956	-0.556706
O	4.364332	-1.755434	2.287157
O	1.871379	1.266699	-2.290079
O	2.558757	2.254693	1.778389
O	5.557493	0.338843	-0.892235
C	-2.544229	-1.431971	-0.866622
C	-1.617592	-1.090182	0.202719
C	-2.569881	0.301824	1.246247
C	-2.378495	1.434173	0.404699
C	-1.048357	1.981504	0.413762
C	-2.674312	-1.040420	-2.178757
C	-3.418885	2.747103	-1.497849
C	4.498699	0.091875	-0.495313
C	-1.056176	3.608163	-1.520808
C	-2.355705	3.544702	-1.978874
C	-3.420631	1.817505	-0.472543
C	-4.296128	-2.483486	-1.671234
C	0.793945	-0.663894	0.758676
C	-4.054879	-1.074818	2.450246
C	-0.277429	-0.699908	-0.144398
C	-3.810130	-1.730150	-2.699894
C	-0.480761	2.907379	-0.431764
C	3.699241	-1.212002	1.513355
C	1.185870	-0.982739	3.135588
C	2.682142	1.279186	1.164430
C	2.613328	-1.912706	-0.808103
C	2.176421	0.664942	-1.349483
H	-1.676965	-1.780442	1.050346
H	-1.917698	0.219790	2.125253
H	-0.414556	1.650982	1.238086
H	-2.018874	-0.357378	-2.712019
H	-4.372337	2.873847	-2.018268
H	-0.387405	4.296693	-2.043670
H	-2.600406	4.194274	-2.824650
H	-4.367033	1.302235	-0.292322
H	-5.128652	-3.174487	-1.579606
H	-5.139945	-1.178345	2.578662
H	-3.608831	-0.739954	3.403500
H	-3.636714	-2.055462	2.171108
H	-0.063612	-0.479630	-1.189337
H	-4.209985	-1.680011	-3.709373
H	0.563117	3.150677	-0.218601
H	0.534955	-1.022850	4.020089
H	1.863402	-0.121149	3.218855
H	1.774332	-1.909537	3.078868



Model compound 3e;

E: -2494,724662 u.a.

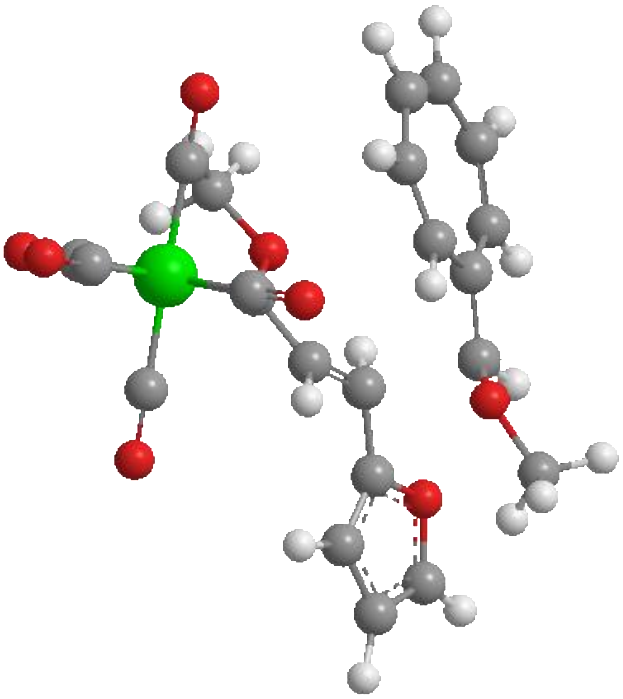
Cr	-0.310990	0.525845	2.278378
O	-0.465565	2.006487	-0.390290
O	0.500267	-2.316780	-2.598223
O	-1.120293	-2.368824	1.795194
O	-2.942109	-0.432525	-0.938132
O	-3.253707	1.295058	2.371015
O	2.594123	-0.369683	2.325432
O	0.583966	3.250552	3.278662
O	-0.484876	-0.199912	5.218778
C	-1.914055	-1.175972	-1.453579
C	-0.714939	-0.393448	-1.859601
C	0.146299	-0.991385	-2.977775
C	1.339394	-0.071065	-2.967319
C	1.567764	0.433376	-1.560718
C	-2.268864	-2.495650	-1.472619
C	3.264852	1.153892	-3.929708
C	-0.419814	0.074762	4.101147
C	4.054925	0.332253	-1.699952
C	4.147795	1.152631	-2.885242
C	2.070528	0.349579	-4.025159
C	-3.949882	-1.291787	-0.629852
C	-0.165742	0.918315	0.290055
C	1.222214	-3.019347	-3.585498
C	0.341924	-0.074956	-0.745975
C	-3.596119	-2.569145	-0.939739
C	2.906900	-0.088064	-1.120861
C	-2.135183	1.023072	2.313300
C	-0.989034	3.192758	0.210842
C	0.235753	2.240233	2.842961
C	-0.826074	-1.264291	1.916814
C	1.496867	-0.021662	2.279914
H	-1.073502	0.579187	-2.234819
H	-0.378868	-1.003370	-3.951918
H	1.595706	1.536818	-1.580186
H	-1.640562	-3.308821	-1.818487
H	3.549677	1.714334	-4.825910
H	5.003329	0.008056	-1.258457
H	5.077855	1.714723	-3.019806
H	1.749405	0.059723	-5.031953
H	-4.839362	-0.840729	-0.201085
H	1.407954	-4.026115	-3.187031
H	2.190977	-2.539138	-3.811596
H	0.642925	-3.107295	-4.525534
H	0.601353	-1.017758	-0.249346
H	-4.203506	-3.459761	-0.800692
H	2.947810	-0.816185	-0.306262
H	-1.286502	3.834463	-0.627175
H	-0.210436	3.689585	0.803057
H	-1.858009	2.962431	0.838041



Model compound TS2;

E: -2494,671036 u.a. (431i)

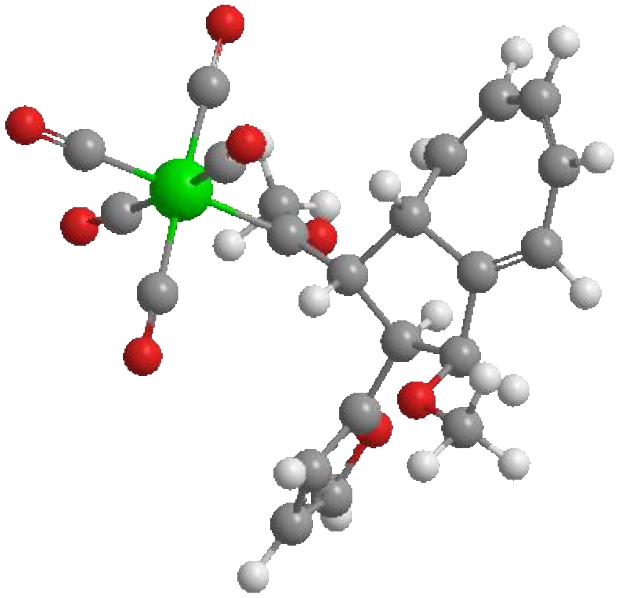
Cr	-2.449949	-0.787036	0.127309
O	-0.301812	0.742570	-1.660390
O	2.936467	0.241074	1.799898
O	-1.259485	-3.608440	0.151596
O	4.150843	-1.291742	-1.239260
O	-3.641385	-1.371432	-2.632333
O	-1.310690	-0.246361	2.909555
O	-3.630112	2.032391	0.221176
O	-5.022315	-1.836755	1.361930
C	2.907624	-1.517724	-0.660558
C	1.969896	-0.394318	-0.659492
C	2.937261	0.880761	0.574064
C	2.071142	2.022272	0.449864
C	2.365990	2.962690	-0.565763
C	2.858395	-2.816009	-0.183738
C	-0.241859	2.815774	1.191351
C	-4.030802	-1.432267	0.881918
C	0.336927	4.482906	-0.621595
C	-0.507089	3.919676	0.329602
C	0.874149	2.000457	1.267903
C	4.869228	-2.455451	-1.116721
C	-0.555376	-0.122336	-0.632679
C	4.187423	-0.350542	2.179389
C	0.658523	-0.619743	-0.104211
C	4.123793	-3.418327	-0.479483
C	1.633223	4.063138	-1.015195
C	-3.156222	-1.123172	-1.595055
C	-1.337845	1.199865	-2.537879
C	-3.158435	0.958091	0.150034
C	-1.710680	-2.528627	0.131540
C	-1.739921	-0.462482	1.838638
H	1.995426	0.203191	-1.580700
H	3.917840	0.932883	0.076543
H	3.334615	2.812794	-1.064261
H	1.995076	-3.288332	0.283417
H	-1.041919	2.578080	1.902602
H	-0.051112	5.365421	-1.146758
H	-1.488389	4.391259	0.455496
H	0.873673	1.244527	2.057409
H	5.867709	-2.436900	-1.549607
H	4.017089	-0.803633	3.167654
H	4.978702	0.420887	2.261928
H	4.505506	-1.135517	1.470357
H	0.588949	-1.289698	0.756382
H	4.434416	-4.440612	-0.264133
H	2.116087	4.671500	-1.789365
H	-0.886043	2.016922	-3.122854
H	-2.208341	1.575779	-1.979665
H	-1.654670	0.392068	-3.218847



Model compound 6e;

E: -2494,721169 u.a

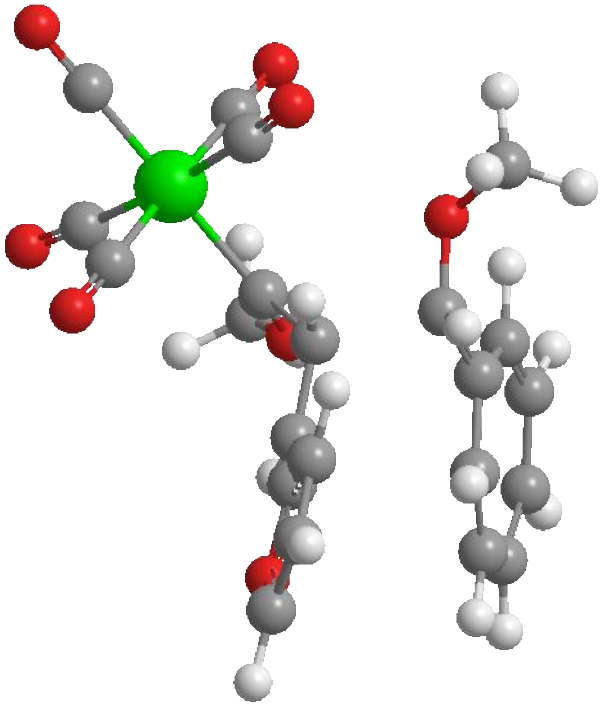
Cr	2.077645	-0.684590	-0.956261
O	0.608695	-0.782470	1.726730
O	-3.336674	0.626327	-0.725970
O	-0.031598	-2.112289	-2.621888
O	-2.357289	-2.267963	2.024583
O	3.118307	-3.392827	-0.055363
O	1.428192	1.900030	-2.416559
O	4.117181	0.801101	0.742700
O	4.117622	-1.030663	-3.174752
C	-2.347530	-1.531390	0.871794
C	-1.904776	-0.117193	1.017637
C	-2.921549	0.958963	0.595853
C	-2.081041	2.215754	0.604975
C	-2.526671	3.490324	0.703042
C	-2.764008	-2.309933	-0.172673
C	0.085265	2.306271	1.681898
C	3.341856	-0.900163	-2.332472
C	-0.452108	4.717415	1.358985
C	0.214582	3.613798	2.005905
C	-0.617551	1.856429	0.428634
C	-2.783360	-3.517140	1.704802
C	0.644984	-0.410837	0.464518
C	-4.390036	1.413141	-1.228878
C	-0.660167	0.313670	0.193709
C	-3.045911	-3.604102	0.370697
C	-1.691180	4.663549	0.786003
C	2.686552	-2.360077	-0.334669
C	1.670594	-1.497341	2.367452
C	3.341579	0.231994	0.107853
C	0.761927	-1.575158	-1.985076
C	1.631835	0.938070	-1.815815
H	-1.689849	0.038728	2.085131
H	-3.801472	1.006027	1.263544
H	-3.608091	3.660451	0.746163
H	-2.859703	-1.988436	-1.204539
H	0.526167	1.553492	2.339891
H	0.006883	5.704871	1.470700
H	0.854850	3.868652	2.857420
H	-0.190432	2.385439	-0.437474
H	-2.844979	-4.221125	2.529137
H	-4.677830	0.977552	-2.195748
H	-4.088992	2.464285	-1.390484
H	-5.268362	1.395323	-0.554295
H	-0.900752	0.174685	-0.868860
H	-3.399969	-4.482364	-0.163298
H	-2.146717	5.611226	0.481450
H	1.430819	-1.471878	3.437089
H	2.638364	-1.017366	2.179346
H	1.681377	-2.535633	2.014194



Model compound TS3;

E: -2494,657996 u.a. (475i)

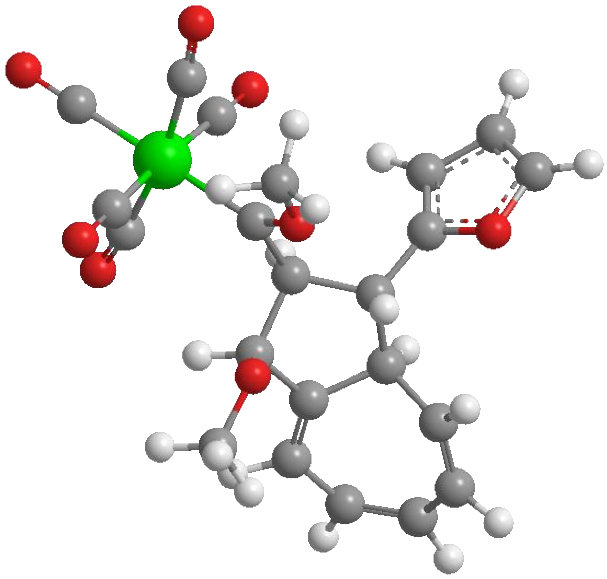
Cr	2.481649	-0.509536	-0.118357
O	-0.380045	-1.057289	-1.131135
O	-0.689050	-1.245399	2.141235
O	2.230324	0.166362	2.832170
O	-2.000374	3.616951	-1.230050
O	2.653971	2.454494	-0.794094
O	2.282130	-3.456763	0.597460
O	3.198527	-1.130455	-3.006102
O	5.469842	-0.586216	0.368316
C	-1.356243	2.881452	-0.265840
C	-1.095672	1.519477	-0.563656
C	-1.494175	-0.298268	1.536323
C	-2.609953	-0.760011	0.769639
C	-3.407043	0.313528	0.189316
C	-1.141868	3.688653	0.843299
C	-3.655507	-2.781868	-0.341637
C	4.331084	-0.557116	0.181824
C	-4.801890	-0.885101	-1.548099
C	-4.529261	-2.216176	-1.294138
C	-2.778841	-2.127785	0.520194
C	-2.183331	4.867972	-0.737854
C	0.450223	-0.369110	-0.371742
C	-0.739208	-1.230855	3.558350
C	-0.381277	0.655098	0.325230
C	-1.677439	4.968567	0.527391
C	-4.320610	0.245144	-0.832672
C	2.576913	1.335565	-0.537704
C	0.051462	-2.091530	-2.015946
C	2.868064	-0.904849	-1.923319
C	2.283783	-0.095700	1.709561
C	2.343931	-2.340714	0.311525
H	-1.353196	1.174397	-1.563914
H	-1.695681	0.579762	2.171135
H	-3.323174	1.281784	0.687138
H	-0.634824	3.400763	1.760439
H	-3.632817	-3.874307	-0.306741
H	-5.518184	-0.674951	-2.346361
H	-5.068510	-2.937497	-1.917570
H	-2.111405	-2.768468	1.104890
H	-2.679250	5.569980	-1.401264
H	-0.029260	-1.990646	3.910095
H	-1.751554	-1.475517	3.927061
H	-0.433353	-0.248315	3.959381
H	0.191519	1.192225	1.086462
H	-1.681967	5.856647	1.154383
H	-4.768749	1.201888	-1.121081
H	-0.865102	-2.606820	-2.327457
H	0.725716	-2.791433	-1.508089
H	0.548762	-1.652354	-2.890623



Model compound 7e;

E: -2494,722550 u.a.

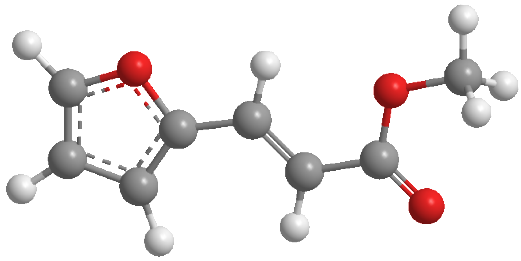
Cr	-2.609025	-0.199389	-0.278252
O	-0.508278	0.696013	1.761749
O	0.917793	-1.829086	1.415600
O	-1.625948	-2.462367	-2.044825
O	2.578148	2.987905	0.818259
O	-1.859963	1.742828	-2.488736
O	-3.210252	-2.212934	1.924266
O	-4.237941	2.000977	1.039749
O	-5.252311	-0.798008	-1.635235
C	1.749149	2.214454	0.057435
C	1.768206	0.759812	0.372106
C	1.020713	-1.504132	0.034533
C	2.446279	-1.408986	-0.454151
C	2.974227	-0.013247	-0.224206
C	1.111566	2.995534	-0.866205
C	4.515118	-2.264478	-1.521301
C	-4.247166	-0.570861	-1.118655
C	5.311576	-0.737165	0.301313
C	5.483138	-1.533548	-0.892820
C	3.131362	-2.365404	-1.121641
C	2.465723	4.267703	0.372057
C	-0.793622	0.203084	0.585229
C	1.271849	-3.162227	1.714093
C	0.536857	-0.038094	-0.115220
C	1.579005	4.335187	-0.658076
C	4.176837	-0.103795	0.673264
C	-2.143863	1.013469	-1.642176
C	-1.490030	1.001736	2.756061
C	-3.562276	1.180385	0.591974
C	-1.931131	-1.601589	-1.339550
C	-2.982781	-1.439605	1.101516
H	1.811514	0.653494	1.465962
H	0.433003	-2.219836	-0.563607
H	3.274378	0.426223	-1.194447
H	0.390957	2.667409	-1.609829
H	4.835155	-2.926238	-2.332332
H	6.181893	-0.665377	0.962523
H	6.511118	-1.663776	-1.246838
H	2.609858	-3.292025	-1.386672
H	3.072151	5.003825	0.890696
H	1.102898	-3.300808	2.790635
H	2.332581	-3.369098	1.486322
H	0.642116	-3.883556	1.158109
H	0.389026	0.123380	-1.194800
H	1.287324	5.227850	-1.205462
H	4.125517	0.377824	1.654972
H	-0.924520	1.136144	3.685675
H	-2.209981	0.182450	2.863525
H	-2.002779	1.935422	2.493512



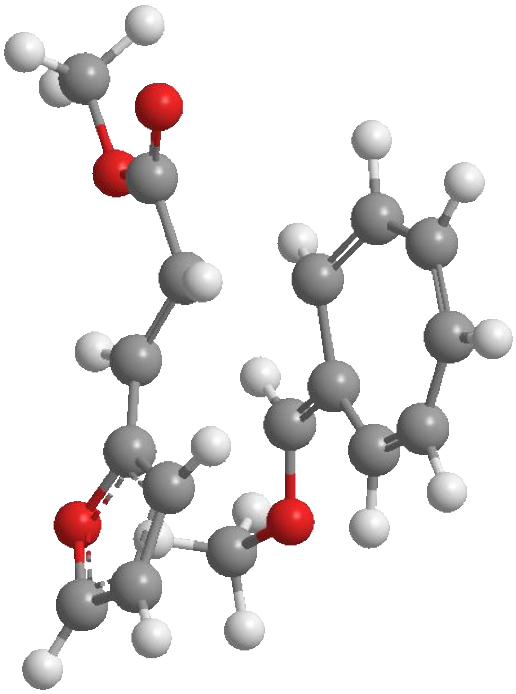
Model compound 8e;

E: -535,051505 u.a.

O	-2.084818	1.634200	-0.000131
O	2.605991	0.244973	0.000568
C	1.493094	-0.553541	0.000121
C	0.230106	0.131760	0.000094
C	1.883917	-1.874631	-0.000210
C	3.685322	-0.564665	0.000517
C	-2.255433	0.291826	-0.000218
C	-0.986675	-0.452038	-0.000272
C	3.306224	-1.879046	0.000051
C	-3.294101	2.391957	-0.000099
H	0.290748	1.223055	0.000405
H	1.223949	-2.738046	-0.000597
H	4.651188	-0.068320	0.000842
H	-1.114352	-1.536290	-0.000578
H	3.966421	-2.742375	-0.000089
H	-2.985603	3.444171	-0.000186
H	-3.897020	2.168366	0.892644
H	-3.897145	2.168243	-0.892725
O	-3.347787	-0.237739	-0.000389



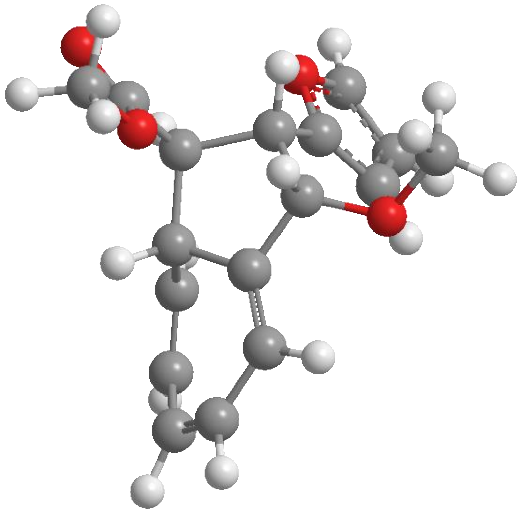
Model compound TS4;



E: -959,894494 u.a. (459i)

O	3.244758	0.238673	-0.340431
O	-1.038270	-1.457532	2.398551
O	-0.540164	-2.936083	-0.643324
C	-0.454111	-1.596711	-0.945452
C	0.733083	-0.922203	-0.593927
C	-0.190717	-0.511055	1.938353
C	-0.640506	0.591441	1.250258
C	0.433495	1.460094	0.692265
C	-1.644986	-1.191524	-1.539181
C	-2.693905	1.714733	0.252738
C	-0.909031	3.449517	-0.145352
C	-2.211765	2.949076	-0.208435
C	-2.017328	0.698975	0.917278
C	-1.756694	-3.367205	-1.059846
C	-0.416748	-2.612676	2.931997
C	0.961109	0.447597	-0.900776
C	-2.473953	-2.347060	-1.615177
C	0.244467	2.814623	0.305320
C	4.600666	0.662528	-0.480651
H	1.538880	-1.517053	-0.163552
H	0.857951	-0.606308	2.239004
H	1.380211	1.308478	1.223426
H	-1.861543	-0.198530	-1.919711
H	-3.766892	1.547155	0.116694
H	-0.774719	4.474855	-0.503579
H	-2.960496	3.617861	-0.644084
H	-2.633124	-0.123458	1.289150
H	-1.964920	-4.420802	-0.898551
H	-1.217956	-3.240987	3.341335
H	0.285790	-2.351826	3.743745
H	0.118487	-3.172153	2.146709
H	0.289718	0.905399	-1.630673
H	-3.475719	-2.416405	-2.031402
H	1.162296	3.405954	0.237209
H	5.183741	0.027168	0.197011
H	4.712787	1.721669	-0.205312
H	4.946494	0.533766	-1.517087
C	2.350698	0.921088	-1.101900
O	2.670721	1.847166	-1.815472

Model compound 9e;



E: -958,956469 u.a.

O	2.378229	-1.240949	1.260124
O	-1.876473	-0.246582	1.700627
O	-1.257432	-1.609749	-2.276679
C	-1.403879	-0.895750	-1.119213
C	-0.331382	-1.125037	-0.103967
C	-0.555910	-0.367115	1.233144
C	0.081099	0.978912	1.014034
C	1.064796	0.911794	-0.128616
C	-2.528243	-0.121849	-1.195168
C	0.410266	3.385068	1.504770
C	0.540630	3.210205	-0.984028
C	0.729595	3.888859	0.274221
C	-0.135629	2.079016	1.768818
C	-2.296101	-1.282006	-3.089617
C	-2.408241	-1.451231	2.205617
C	1.044900	-0.565438	-0.594267
C	-3.108315	-0.374286	-2.481470
C	0.583171	1.872744	-1.184005
C	3.470645	-1.978373	1.817122
H	-0.253107	-2.212629	0.059405
H	0.049037	-0.900560	1.995122
H	2.070307	1.219427	0.209920
H	-2.888899	0.541622	-0.416397
H	0.455043	4.074981	2.353961
H	0.307801	3.845572	-1.845597
H	1.012088	4.945426	0.224325
H	-0.794409	1.975512	2.636836
H	-2.314519	-1.779579	-4.054502
H	-3.388982	-1.213650	2.639924
H	-1.760576	-1.880171	2.995083
H	-2.549147	-2.209499	1.413293
H	1.114460	-0.650961	-1.685791
H	-4.013356	0.063769	-2.894740
H	0.282668	1.467780	-2.155270
H	3.471766	-1.744026	2.887988
H	4.420194	-1.671849	1.355167
H	3.334644	-3.057963	1.657663
C	2.208736	-1.382013	-0.074041
O	2.911696	-2.091993	-0.753621