Electronic Supplementary Information [ESI]

Solar driven uphill conversion of dicyclopentadiene to cyclopentadiene: an important synthon for energy systems and fine chemicals

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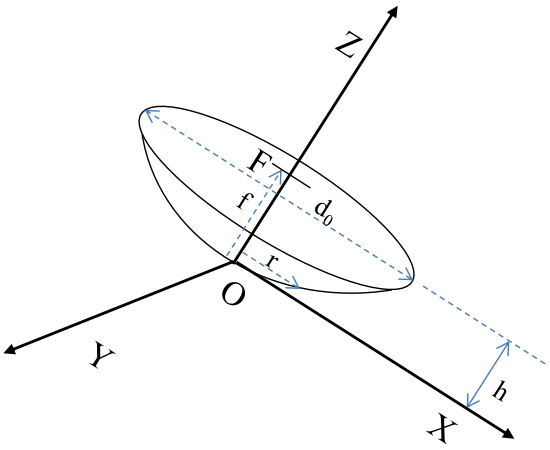
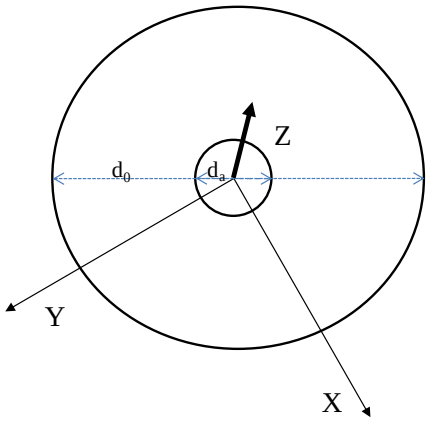
Table of Contents

Description of parabolic dish concentrator employed for synthesis of cyclopentadiene (Cp) from dicyclopentadiene (5)

The reaction was carried out in a solar parabolic dish concentrator constructed to bring about temperature of about 200°C to 250 °C at the focus. The concentration ratio at the focus was calculated to be 20 *X*. Accordingly the parabola had the opening diameter (d_0) of 1.38 m and focal length (f) of 0.34 m. The height (h) of the parabolic dish concentrator was 0.35 m. It was a semi-circular trough made of poly-vinyl chloride plastic with small mirrors fixed on it to collect solar rays onto the focus where the glass round bottom flask was placed. The collector aperture area was 1.83 m^2 and the cross section of the opening of the parabola was 1.49 m^2. The dish had to be tracked according to the day long solar movement to get the maximum solar radiation on the flask at all times.





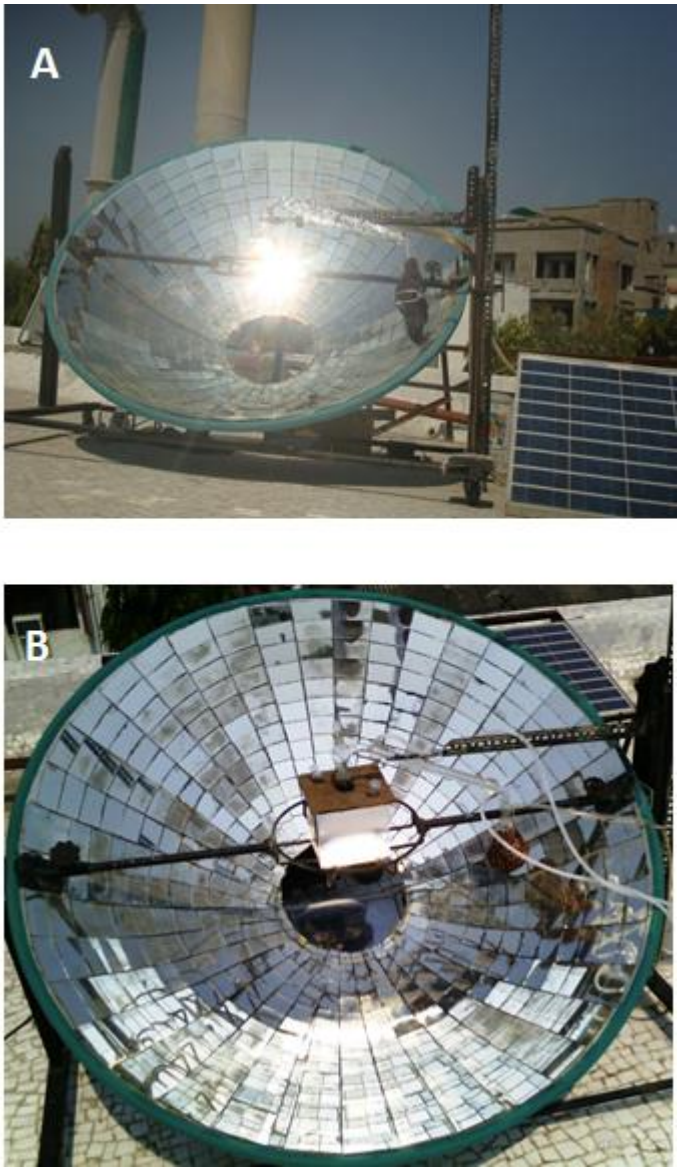


Fig. S1 Experimental set-up for solar synthesis of Cp from 5 for (A) entries 1 and 2, Table 2, and (B) entry 3, Table 2. The only difference between (A) and (B) was that in the latter case the glass RB flask was painted black and inserted in a wooden box with transparent glass at the bottom and other interiors of the box painted black.

Description of offset parabola employed for the synthesis of 7

An offset parabolic type of solar dish collector with width of 0.62 m, diameter of 0.68 m and depth of 0.05 m was fabricated. 24 pieces of anodized aluminum reflector were joined in such a way that the focus was at 0.43 m. The concentration ratio was calculated to be 59 *X* to achieve a maximum temperature of 200 ^{o}C at the focus considering the ambient conditions prevailing.

Fig. S2 Picture of experimental set-up for synthesis of 7

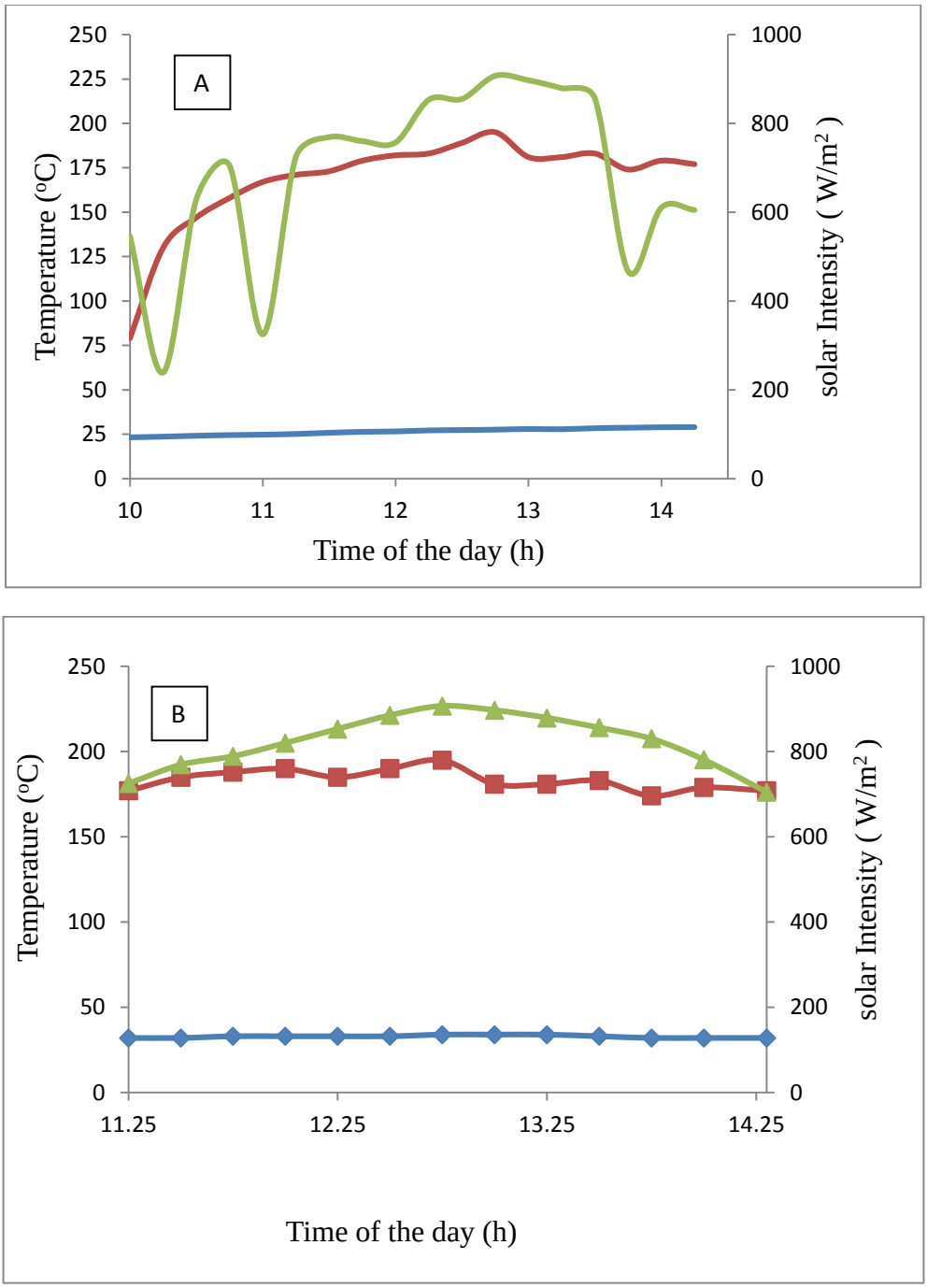


Fig. S3 Global insolation (green), ambient temperature (blue) and reaction temperature (red) recorded during the reactions of (A) Entry 2, Table 2 and (B) Entry 3, Table 2.

Table S1 Other weather related measurements during the reaction of Entry 2, Table 2.

Time/ HH:MM	Wind Speed/ m sec^{-1}	Wind Dir./°	Atm. Pressure/ mBar
10:15	4.1	71	1010.1
10:45	5.7	86	1010.1
11:15	3.7	44	1010.1
11:45	4.6	76	1010.1
12:15	5.7	89	1010.1
12:45	4.7	69	1009
13:15	5.6	57	1009
13:45	5.6	41	1007.9
14:15	5.7	21	1007.9

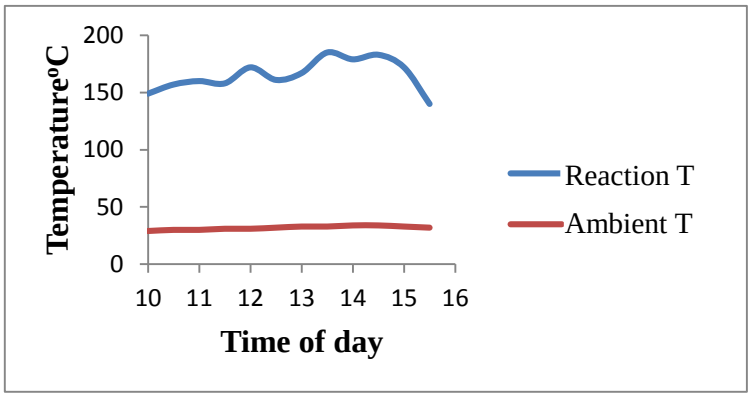
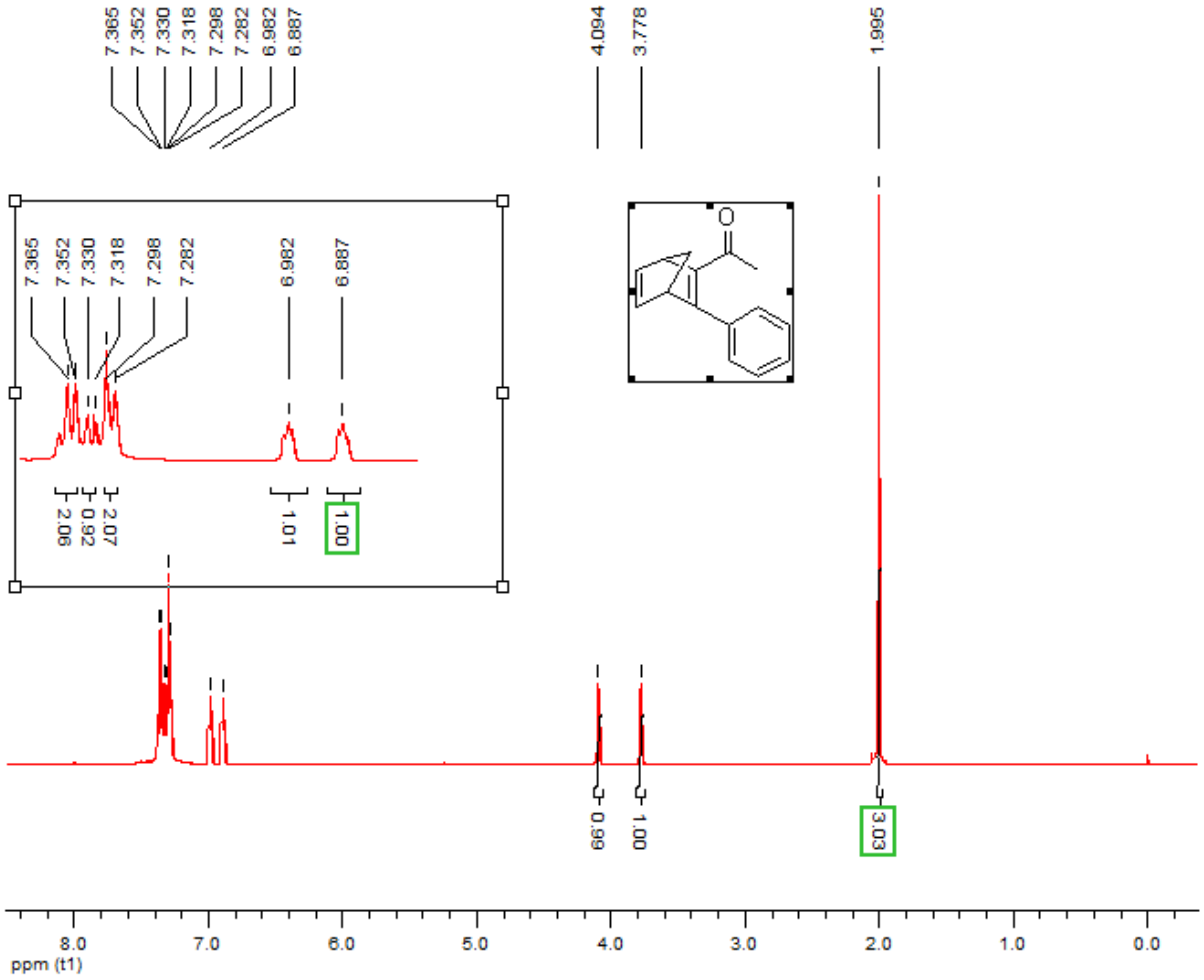


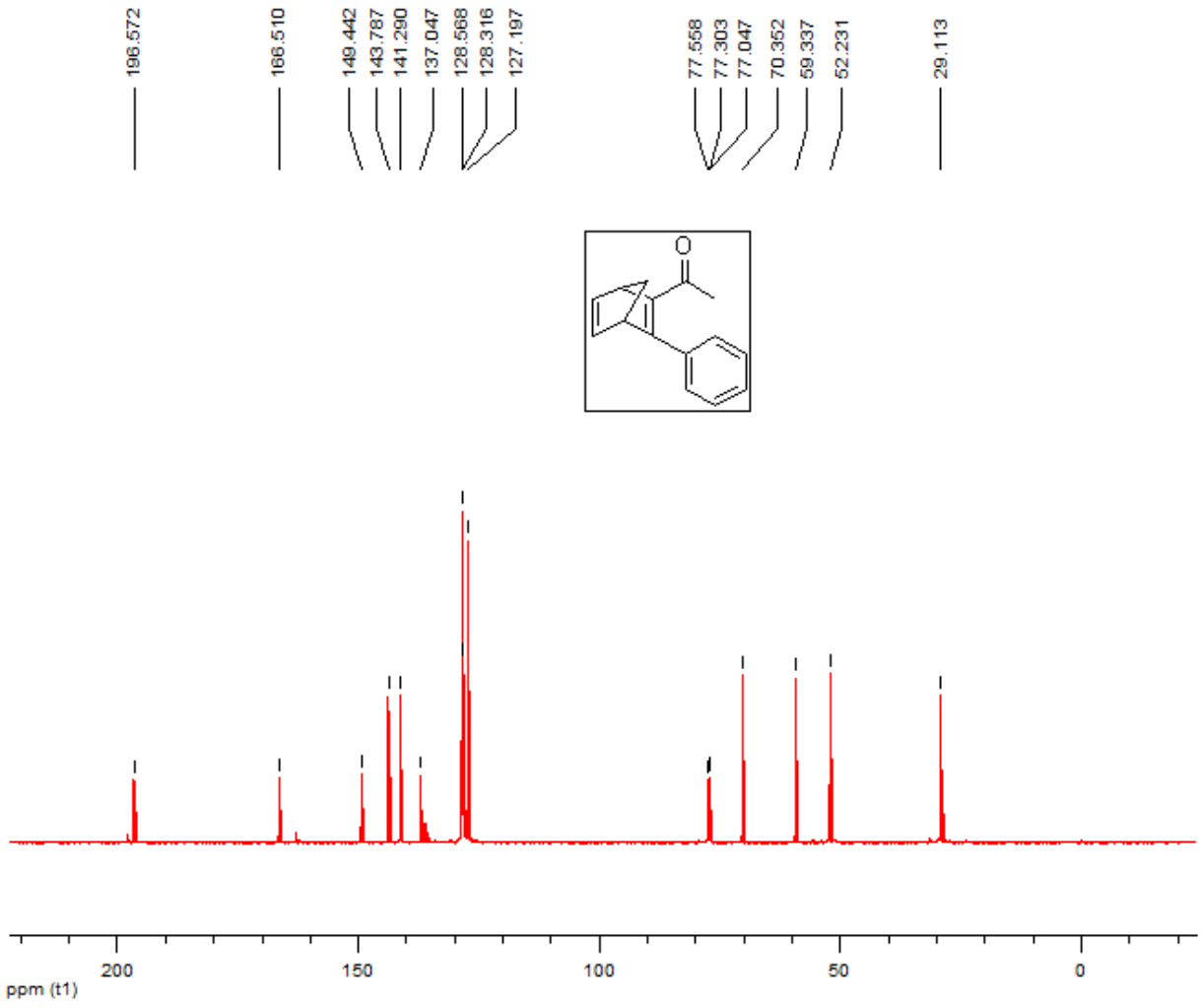
Fig. S4 Temperature profile during the reaction of eqn. 5

Solar mediated synthesis of 1-(3-phenylbicyclo[2.2.1]hepta-2,5-dien-2-yl) ethanone (7)

^{1}H NMR



^{13}C NMR

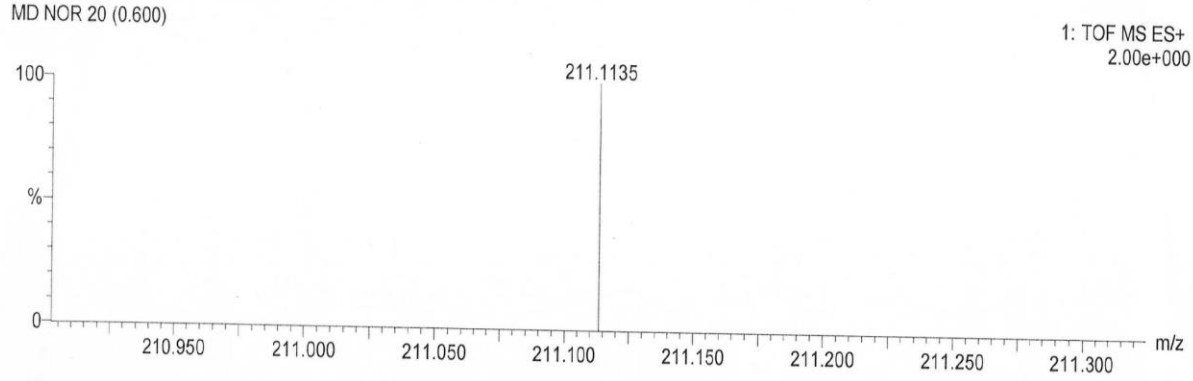

196.572
166.510
149.442
143.787
141.290
137.047
128.568
128.316
127.197
77.558
77.303
77.047
70.352
59.337
52.231
29.113
O
200
150
100
50
0
ppm (t1)

HRMS of 1-(3-phenylbicyclo[2.2.1]hepta-2,5-dien-2-yl) ethanone (7)

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

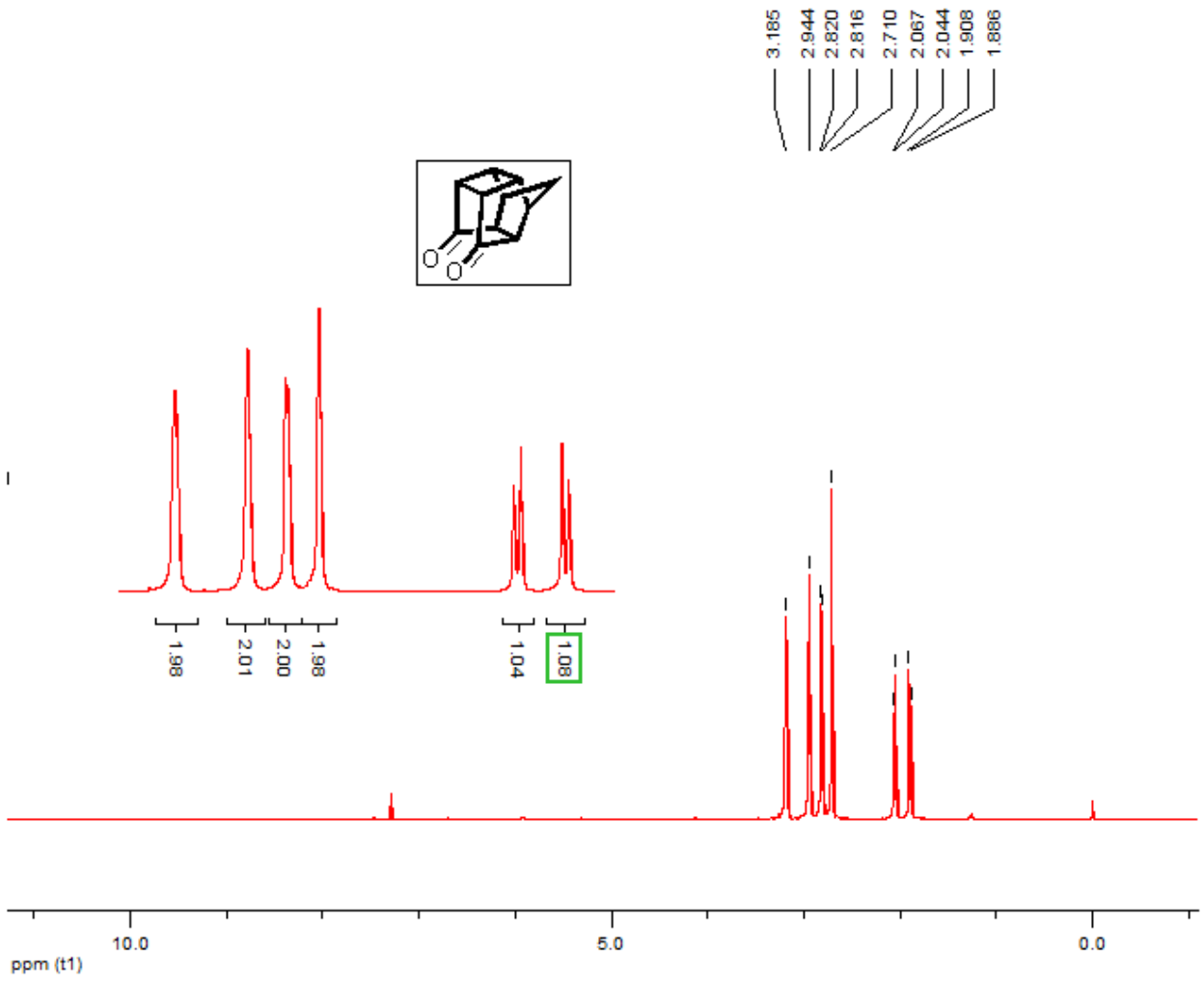
Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-16 H: 0-15 O: 0-1 P: 0-1
MD NOR
MD NOR 20 (0.600)



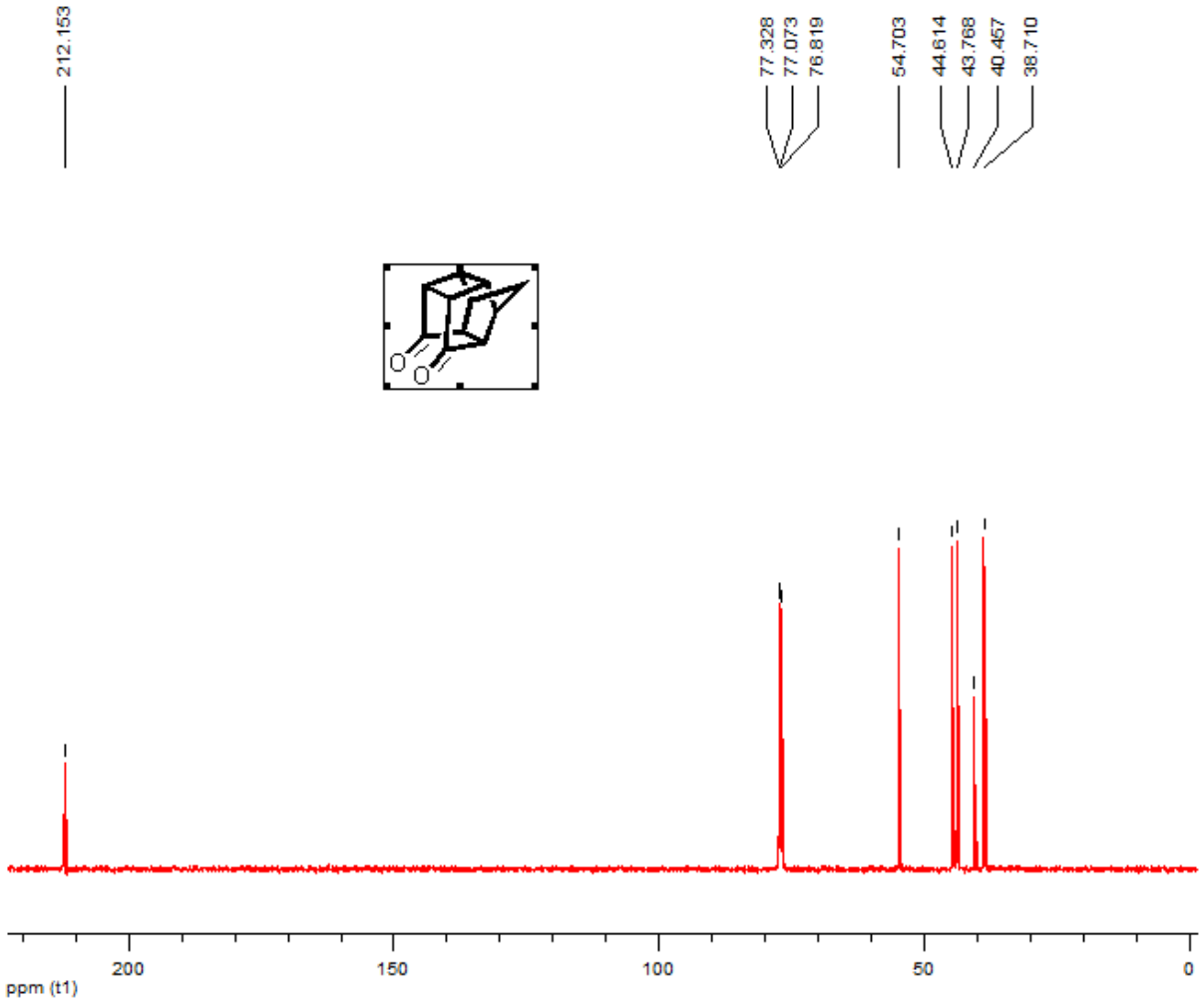
Minimum:				-1.5		
Maximum:		5.0	50.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
211.1135	211.1123	1.2	5.7	8.5	n/a	C15 H15 O

Solar mediated synthesis of Pentacyclo-[5.4.0.0^{2,6}.0^{3,10}. 0^{5,9})undecan-8, 11–dione (9)

^{1}H NMR



^{13}C NMR


212.153
77.328
77.073
76.819
54.703
44.614
43.768
40.457
38.710
O
O
200
150
100
50
0
ppm (t1)

xyz co-ordinates of compounds optimized at CBS-QB3 level of theory. Free energy (G) and enthalpies (H) are given in Hartree unit.

Compound-1

H=-270.94132

G=-270.97102

C	1.24285500	0.66619200	-0.52113000
C	0.00000000	1.12243200	0.27316600
C	0.00000000	-1.12243200	0.27316600
C	1.24285500	-0.66619200	-0.52113000
H	1.93133000	1.33385500	-1.02110500
H	1.93133000	-1.33385500	-1.02110500
C	0.00000000	0.00000000	1.35623600
H	-0.89884300	0.00000000	1.97671600
H	0.89884300	0.00000000	1.97671600
C	-1.24285500	0.66619200	-0.52113000
H	-1.93133000	1.33385500	-1.02110500
C	-1.24285500	-0.66619200	-0.52113000
H	-1.93133000	-1.33385500	-1.02110500
H	0.00000000	2.15750000	0.61134900
H	0.00000000	-2.15750000	0.61134900

Compound-2

H=-270.9049

G=-270.93477

C	0.77513100	-0.70934700	0.75797600
C	1.15208600	0.55070200	0.00012000
C	-1.15208600	0.55070200	-0.00012400
C	-0.77491300	-0.70892000	0.75841800
H	1.42529400	-1.23032600	1.44691200
H	-1.42519800	-1.22934400	1.44765600
C	0.00000100	1.53792700	-0.00000300

Compound-7

H=-653.98389

G=-654.0316

C	-1.24061900	0.45290800	0.22863100
C	-2.50262400	-0.44212100	0.36478300
C	-0.74364200	-1.80888100	0.48643800
C	-0.16361700	-0.37916000	0.29703300
C	-1.94979500	-1.45766500	1.39782800
H	-2.61465600	-2.30707100	1.56623800
H	-1.66056100	-0.99883900	2.34568500
C	-2.56169300	-1.36080600	-0.87099600
C	-1.50988200	-2.17515700	-0.79849200
H	-3.42351300	0.07950200	0.61644200
H	-0.03243600	-2.54612700	0.85178500
H	-3.30001800	-1.29184300	-1.65846000
H	-1.18829800	-2.92044200	-1.51315900
C	-1.32834900	1.88737500	-0.10388400
O	-0.44319500	2.69538000	0.12701300
C	-2.61807900	2.35362100	-0.76735800
H	-2.93630100	1.67769600	-1.56549400
H	-3.42741300	2.39455200	-0.03086800
H	-2.45981200	3.35441200	-1.16660500
C	1.27846600	-0.17788000	0.13010600
C	1.93780500	1.00557300	0.51009500
C	2.05504400	-1.22233100	-0.41088800
C	3.31267000	1.13442000	0.34305400
H	1.35900100	1.81874600	0.92018300
C	3.42549700	-1.08187300	-0.58967900

H	0.00009300	2.17576000	-0.88997000
H	-0.00009100	2.17575900	0.88996500
C	0.77491200	-0.70892500	-0.75841500
H	1.42519900	-1.22935200	-1.44764900
C	-0.77513100	-0.70935100	-0.75797200
H	-1.42529700	-1.23033300	-1.44690400
H	2.18544800	0.87555400	0.00010000
H	-2.18544700	0.87555600	-0.00010800

Compound-5

H=-387.45403

G=-387.48887

C	-1.09630300	1.11655400	-0.17747700
C	-1.02634600	-1.14221600	-0.14713900
C	-1.91677700	-0.04728400	-0.78656400
H	-1.90542400	-0.06108100	-1.88105100
H	-2.94745900	-0.07436800	-0.42703000
C	0.31395400	0.79843900	-0.81696100
H	0.32241600	1.19710600	-1.83763300
C	0.35931700	-0.77379600	-0.79131700
H	0.38941500	-1.17849200	-1.80510400
H	-1.45120500	2.13019500	-0.36473900
H	-1.32599700	-2.17925300	-0.30219800
C	1.64448100	-1.15887000	-0.01225900
H	1.43118500	-1.77792400	0.86747100
H	2.33617100	-1.73991200	-0.63330600
C	-1.05145100	0.67699700	1.27685500
H	-0.95775000	1.34344400	2.12474300
C	-1.01308000	-0.65890500	1.29635300
H	-0.89093700	-1.29333400	2.16503900
C	2.24811600	0.16870200	0.38235700
H	1.57756100	-2.14611500	-0.71456300
C	4.06228500	0.09820300	-0.20898700
H	3.80028800	2.05377800	0.64763700
H	3.99754400	-1.89505200	-1.02237100
H	5.13336900	0.20641500	-0.33865800

Compound-8

H=-574.61023

G=-574.65111

C	-0.13463700	-0.77963100	-0.82320100
C	-1.49723300	-1.12871600	-0.10223000
C	-1.49673900	1.12920100	-0.10204800
C	-0.13438400	0.77971000	-0.82323100
C	-2.38857500	0.00047700	-0.66606800
H	-3.38775600	0.00065600	-0.22743100
H	-2.46211800	0.00056800	-1.75772700
C	-1.35718800	-0.66867200	1.34180100
C	-1.35662600	0.66882700	1.34188300
H	-1.80736600	-2.15935600	-0.25752400
H	-1.80646100	2.15999800	-0.25712100
H	-1.18646700	-1.32638300	2.18421200
H	-1.18542700	1.32629400	2.18439000
C	1.05549200	1.48644500	-0.19901100
C	1.05491400	-1.48672700	-0.19877600
C	2.18882700	-0.67090100	0.29819600
C	2.18905700	0.67025200	0.29815700
O	1.08878100	-2.69940400	-0.10888100
O	1.08952700	2.69908500	-0.10869600
H	-0.18987700	-1.15489800	-1.85000300
H	-0.18966400	1.15499400	-1.85002300

H	3.16168800	0.24036800	0.96350300
C	1.54316900	1.21101100	-0.05471200
H	1.80741700	2.24946000	0.11548500

Acetylene

H=-77.18406

G=-77.20449

C	0.00000000	0.00000000	0.59902600
H	0.00000000	0.00000000	1.66135000
C	0.00000000	0.00000000	-0.59902600
H	0.00000000	0.00000000	-1.66135000

Cyclopentadiene

H= -193.70833

G=-193.73674

C	1.17915800	-0.28195800	0.00027000
C	-0.00100500	-1.21569400	-0.00008400
C	-1.17961700	-0.28001500	0.00010300
C	-0.73352200	0.98998800	0.00008900
C	0.73515600	0.98878600	-0.00035400
H	-0.00159500	-1.87748900	0.87681200
H	-0.00152100	-1.87728200	-0.87714500
H	2.20975600	-0.60950800	0.00045100
H	1.34892300	1.88064400	-0.00057800
H	-1.34582700	1.88284900	0.00012600
H	-2.21075400	-0.60586000	0.00019100
H	3.02539800	-1.24159600	0.68953200
H	3.02581100	1.24067900	0.68949200

Compound-9

H=-574.62672

G=-574.66397

C	0.91294800	-0.78082200	1.16474300
C	1.35499200	-1.13263600	-0.29358100
C	1.35498200	1.13264800	-0.29359300
C	0.91293800	0.78084800	1.16474000
H	1.45543300	-1.30285000	1.95113800
H	1.45543100	1.30289500	1.95111700
C	2.32768900	0.00000500	-0.64536700
H	2.63454800	-0.00000400	-1.69451500
H	3.22415100	0.00001000	-0.01725200
C	0.06246600	-0.79899400	-1.09048000
C	0.06246400	0.79900200	-1.09047900
H	1.71021500	-2.15419000	-0.43302000
H	1.71021100	2.15420000	-0.43303000
C	-1.03968100	1.31646300	-0.16550500
C	-1.03964000	-1.31650200	-0.16549300
C	-0.64909900	0.79395900	1.21122100
C	-0.64909600	-0.79394500	1.21122600
O	-1.96984100	2.02355600	-0.45340400
O	-1.96980900	-2.02358500	-0.45339400
H	-1.16850100	-1.27562300	2.03578200
H	-1.16850700	1.27563800	2.03577500
H	-0.00078600	1.21647200	-2.09310900
H	-0.00077000	-1.21646400	-2.09310900