

Physico-Chemical Study of Some Cross Conjugated Systems, Part II

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الملخص

يتضمن البحث دراسة لتكاثف سلاسل متعددة من مركبات الإينون ذات الإقتران المتقاطع الحاوية على اصرتين و ثلاث و أربع أوامر $C = C$ مع المينثون تحت ظروف تقنية التحفيز بانتقال الطور (PTC) للحصول على مركبات جديدة تم تشخيصها بالطرق الطيفية. ولغرض وضع ميكانيكيه محتمله لهذه التفاعلات تمت دراسة الحسابات النظرية لكل من هذه التكاثفات باستعمال طريقتي الميكانيك الجزيئي وميكانيك الكم و كذلك لتوضيح الطبيعة الإستثنائية لمركبات الإقتران المتقاطع فضلا عن وضوح تأثير المعوضات على التوزيع الألكتروني للسلسلة الداخلية وعلى توجيهه بالإضافة النيوكلوفيلية والشكل الفراغي ثلاثي الأبعاد للمواد الأولية والنواتج.

Abstract

A series of cross-conjugated enones [1-10] are condensed with menthone under (PTC) technique. The structures of the new products [11-20] were identified by spectral analysis. The probable reaction mechanism for each condensation is investigated by theoretical approach using both quantum mechanic (AM1) and molecular (MM2) computational methods. The unique behavior of these cross conjugated enones toward nucleophilic addition orientation, substituent effect on the electronic distribution, and the polarity of the molecules have been examined.

Introduction

Molecules with cross conjugated bond systems are of great interest for both theoretical and applied chemistry¹⁻². Extended cross-conjugated enones (α, β, γ , and δ) system is an important system due to its presence in biologically active compounds¹⁻⁴. Some of cross conjugated dienones are in pre-clinical trials as anticancer agents, Also extended enones are well known as common flavor constituent in tea, tobacco & foods⁴. In addition, this system has been used as useful substances or intermediates in the synthesis of vitamins⁵ and natural products⁶.

Several theoretical investigations have carried out on a series of cross conjugated compounds^{1,7-9}. Semi-empirical calculations on cyclopentadienone and cyclohexadienone have been reported⁷. The calculation of geometries by empirical force field showed that the rings are planar for both compounds. Electrochemical data and AM1 calculations on a series of cross-conjugated p-phenylene vinylidene with one to four double bonds revealed that electronic interaction between the repeating C=C bond unit is not very strong⁸. Theoretical calculations by the ZINDO method on cross conjugated 2,6-di-(phenylethynyl)pyridine & 2,6-d-(phenylbutadienyl)pyridine showed that the central group in cross-conjugated compound is conjugated with one or the other double bond, but not with both simultaneously⁹.

In conjunction to our interest in the synthesis and condensation reactions of α - β - unsaturated carbonyl compounds with various C-H acids under phase transfer catalysis (PTC)¹⁰⁻¹², the condensation of a series of cross-conjugated enones, dienones [1-3], trienones [4-7], and tetraenones [8-10] with menthone have been investigated. Theoretical calculations using (AM1)¹³ and (MM2)¹⁴ computational method on both reactants & products are performed.

Experimental

1. Instrumental

Melting points were measured using electro thermal (IA9000) digital-series M.P. apparatus. IR spectra were recorded on Tensor-27 Bruker (FT.IR) and U.V spectra were measured by Shimadzu UV-160 spectrophotometer.

2. The Computation

Chemoffice (version 5.0) software package was used for theoretical calculations. Geometrical optimization of dihedral angle, heat of formation (H.F), net atomic charge & bond distance were calculated using Semi-empirical methods (AM1 with package MOPAC). Whilst, MM2 were used for molecular mechanics calculations of steric energy (S.E) and atomic steric energy (A.S.E).

Preparations

1. Preparation of the starting materials

The cross-conjugated enones [1-10] were prepared by standard methods¹⁵⁻¹⁷ where the desired benzaldehyde was condensed with the proper ketone in aqueous ethanolic sodium hydroxide. These enones were identified by their physical & spectral data¹¹⁻¹² (IR, UV, NMR). These data are reported & published¹² in our study of the same series of enones in part(I).

2. General procedure for the condensation of the enones [1-10] with menthone under (PTC)¹⁸.

A mixture of (3ml) 50% NaOH, (25ml) benzene, (0.3gm) benzyl tributylammouium chloride (TEBA) and ((0.0025 mole) of menthone is stirred magnetically for (5min). The enone [1-10] (0.0025 mole) was added dropwise, stirring is continued for certain intervals at 30-40 °C until no further change in color is observed. The benzene layer was separated, washed with water, dried over MgSO₄ and evaporated. The residue obtained is recrystallized from (95%) ethanol.

Table (1) illustrates weight of reactants, time of reactions, names of the products, [11-20], M.P and % yields.

Table (1): Weight of reactants, time of reactions, names of the products, melting points and percentage yields [11-29]

Compd No.	Wt. of Reactants (gm)		X	Time of reaction (min)	Name	m.p & color	Yield %
	Uns. Ketone	Menthone					
11	0.585	0.385	H	90	2-(3-oxo-1,5-diphenylpent-4-enyl)-6-isopropyl-3-methylcyclohexanone	153-155 yellow-orange	43
12	0.670	0.385	Cl	120	2-(5-(p-chlorophenyl)-3-oxo-1-phenylpent-4-enyl)-6-isopropyl-3-methylcyclohexanone	140-142 yellow	50
13	0.620	0.385	CH ₃	90	2-(5-(p-tolyl)-3-oxo-1-phenylpent-4-enyl)-6-isopropyl-3-methylcyclohexanone	164-166 yellow	48

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14	0.56 0.385	Ar = 2-Furyl	120	2-(1-(furan-2-yl)-3-oxo-5-phenylpent-4-enyl)-6-isopropyl-3-methylcyclohexanone	205-208 yellow	39
15	0.650 0.385	H	90	2-(3-oxo-1,7-diphenylhepta-4,6-dienyl)-6-isopropyl-3-methylcyclohexanone	168-170 yellow	51
16	0.730 0.385	Cl	90	2-(1-(p-chlorophenyl)-3-oxo-7-phenylhepta-4,6-dienyl)-6-isopropyl-3-methylcyclohexanone	172-174 yellow	57
17	0.685 0.385	CH ₃	120	2-(1-(p-tolyl)-3-oxo-7-phenylhepta-4,6-dienyl)-6-isopropyl-3-methylcyclohexanone	168-170 yellow	60
*18	0.715 0.385	-----	90	2-(5-oxo-1,9-diphenylnona-1,6,8-trien-3-yl)-6-isopropyl-3-methylcyclohexanone	160-162 yellow	55
**19	0.785 0.385	-----	90	2-(2,8-dimethyl-5-oxo-1,9-diphenylnona-1,6,8-trien-3-yl)-6-isopropyl-3-methylcyclohexanone	177-179 yellow	50
***20	0.750 0.385	-----	90	2-(2-methyl-5-oxo-1,9-diphenylnona-1,6,8-trien-3-yl)-6-isopropyl-3-methylcyclohexanone	168-171 yellow	48

* Ra, Rb = H

** Ra, Rb = CH₃

*** Ra = CH₃, Rb = H

Results and discussion

The condensations of the cross conjugated enones [1-10] with menthone under (PTC) conditions were carried out and the products [11-20] were obtained. The products were identified by the analysis of their IR and UV spectral data. The spectral data of the condensation products are illustrated in table (2). As a representative model of the condensation products, compound [20] is selected. The IR spectrum shows a broad absorption band at (1705-1680cm⁻¹) which is attributed to the stretching vibration of the cyclic & acyclic C=O group overlapped with each other. The absorption at (1600-1585cm⁻¹) belong to (C=C) of the olefinic and aromatic double bond. The isopropy group shows a

strong doublet at (1397-1370 cm^{-1}) due to the inplane and out of plane deformation of the two methyl of menthone fragment.

The UV spectrum of the product [20] exhibits a maximum absorption at λ_{max} (348nm) / with a blue shift when compared with λ_{max} of the reactant [10] (λ_{max} 387nm). The decrease in λ_{max} is due to the decrease in conjugation of the product [20] (table 2).

Table (2): The IR and UV spectral data of products [11-20]

Comp. No.	IR (KBr) cm^{-1}		UV CHCl_3 λ_{max} (nm)
	Band	Interpretation	
11	1712 (s)	$\nu_{\text{C=O}}$ of cyclohexane	322
	1667 (s)	$\nu_{\text{C=O}}$ of unsat. ketone	
	1610 (s)	$\nu_{\text{C=C}}$ olefinic and skeletal vib. of $\text{C}=\text{C}$ aromatic	
	1606 (s)		
	1575 (s)		
	1364-1382 (s)	Gem dimethyl	
	2991 (m)	$\nu_{\text{C-H}}$ of alkane	
3039 (m)	$\nu_{\text{C-H}}$		
12	1679 (s)	$\nu_{\text{C=O}}$ of cyclohexane	314
	1653 (s)	$\nu_{\text{C=O}}$ of unsat. ketone	
	1602 (s)	$\nu_{\text{C=C}}$ olefinic and skeletal vib. of $\text{C}=\text{C}$ aromatic	
	1577 (s)		
	1541 (s)		
	1363, 1356 (s)	Gem dimethyl	
	2870 (w)	$\nu_{\text{C-H}}$ of alkane	
3058 (m)	$\nu_{\text{C-H}}$		
13	1722 (s)	$\nu_{\text{C=O}}$ of cyclohexane	318
	1663 (s)	$\nu_{\text{C=O}}$ of unsat. ketone	
	1603 (s)	$\nu_{\text{C=C}}$ olefinic and skeletal vib. of $\text{C}=\text{C}$ aromatic	
	1588 (s)		
	1568 (s)		
	1377, 1371 (s)	Gem dimethyl	
3011 (m)	$\nu_{\text{C-H}}$ of alkane		
14	1743 (s)	$\nu_{\text{C=O}}$ of cyclohexane	306
	1689 (s)	$\nu_{\text{C=O}}$ of unsat. ketone	
	1240 (s)	$\nu_{\text{C-O}}$ asymmetric str.	
	1612 (s)	$\nu_{\text{C=C}}$ olefinic and skeletal vib. of $\text{C}=\text{C}$ aromatic	
	1593 (s)		
	1564 (s)		
	1391, 1362 (s)	Gem dimethyl	
	2975 (w)	$\nu_{\text{C-H}}$ of alkane	
	3004 (m)	$\nu_{\text{C-H}}$	
3123 (m)	ν_{CH} of furan		
810 (s)	$\nu_{\text{C=O}}$ out of plane (bending of furan)		

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15	1706 (s)	$\nu_{C=O}$ of cyclohexane	308
	1679 (s)	$\nu_{C=O}$ of unsat. ketone	
	1628 (s) 1603 (s) 1582 (s)	$\nu_{C=C}$ olefinic and skeletal vib. of C \cdots C aromatic	
	1352, 1343 (s)	Gem dimethyl	
	2998, 2903 (m)	ν_{C-H} of alkane	
	3014 (m)	ν_{C-H}	
	16	1712 (s)	
1683 (s)		$\nu_{C=O}$ of unsat. ketone	
1608 (s) 1591 (s) 1562 (s)		$\nu_{C=C}$ olefinic and skeletal vib. of C \cdots C aromatic	
1381, 1321 (s)		Gem dimethyl	
2983, 2899 (m)		ν_{C-H} of alkane	
3001 (m)		ν_{C-H}	
17		1726 (s)	$\nu_{C=O}$ of cyclohexane
	1678 (s)	$\nu_{C=O}$ of unsat. ketone	
	1613 (s) 1586 (s) 1574 (s)	$\nu_{C=C}$ olefinic and skeletal vib. of C \cdots C aromatic	
	1385, 1329 (s)	Gem dimethyl	
	2762, 2891 (m)	ν_{C-H} of alkane	
	3026 (m)	ν_{C-H}	
	18	1711 (s)	$\nu_{C=O}$ of cyclohexane
1659 (s)		$\nu_{C=O}$ of unsat. ketone	
1603 (s) 1584 (s)		$\nu_{C=C}$ olefinic and skeletal vib. of C \cdots C aromatic	
1363, 1324 (s)		Gem dimethyl	
2972, 2830 (w)		ν_{C-H} of alkane	
3018 (w)		ν_{C-H}	
19		1663-1699 (br)	$\nu_{C=O}$ of two carbonyl overlapped
	1604 (s) 1571 (s) 1543 (s)	$\nu_{C=C}$ olefinic and skeletal vib. of C \cdots C aromatic	
	1356, 1341 (s)	Gem dimethyl	
	2912, 2823 (m)	ν_{C-H} of alkane	
	3008 (m)	ν_{C-H}	
	20	1680-1705 (br)	$\nu_{C=O}$ of two carbonyl overlapped
1600-1585 (s)		$\nu_{C=C}$ olefinic and skeletal vib. of C \cdots C aromatic	
1370-1397 (s)		Gem dimethyl	
2973, 2880 (w)		ν_{C-H} of alkane	
3056, 3025 (m)		ν_{C-H}	

The proposed mechanism for these reactions is illustrated in Scheme (1). The condensation of 2-methyl-1,9-diphenylnona-1,3,6,8-tetraen-5-one [10] with menthone is selected as a representative model for the possible pathways of the nucleophilic addition process.

Theoretical investigation using CS ChemOffice V. 5 programme on the cross conjugated enones [1-10] and their corresponding addition products [11-20] with menthone have been carried out. The theoretical data, heat of formation (H.F), steric energy minimized by AMI method

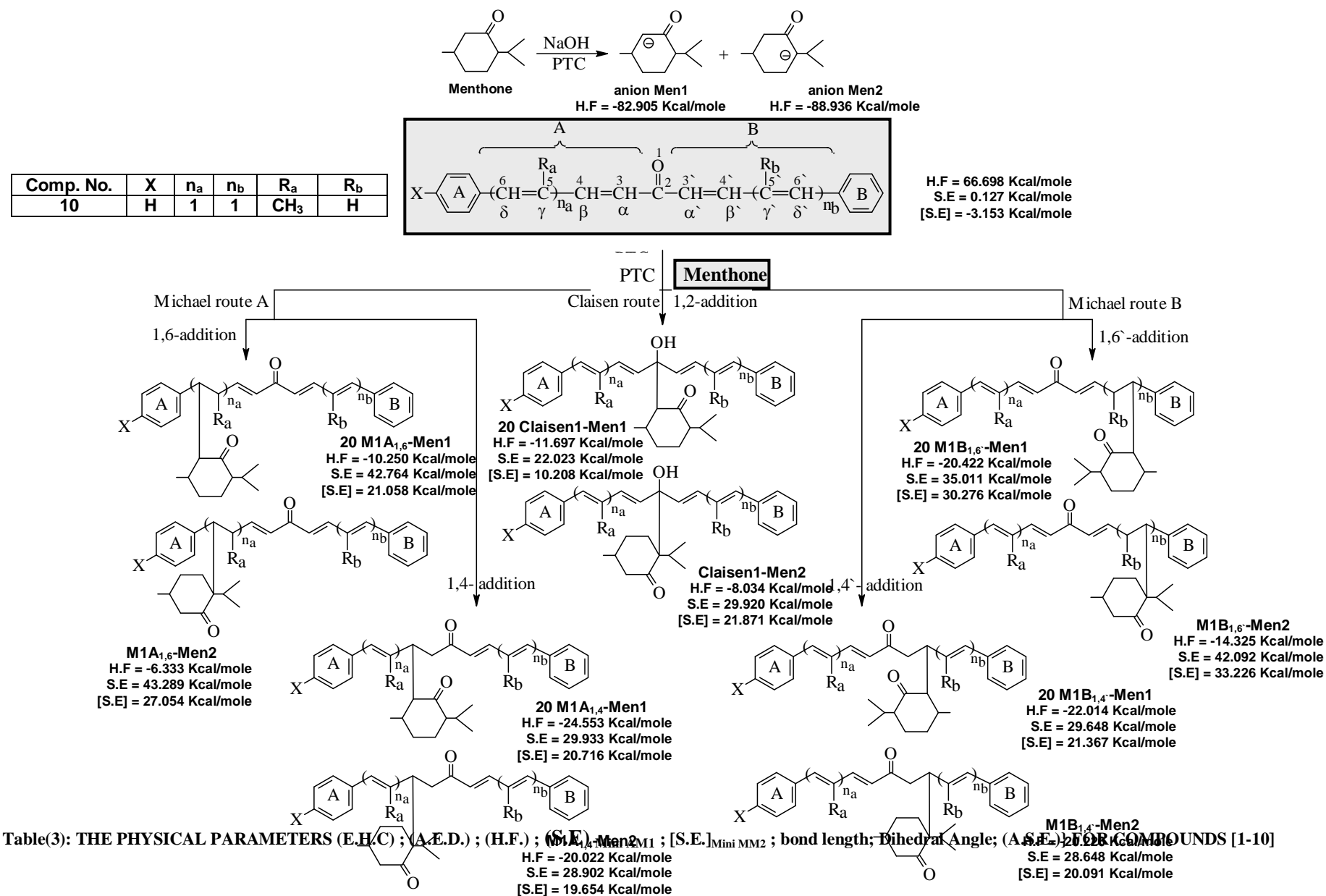
($S.E_{\min z AM1}$) and steric energy minimized by MM2 ($S.E_{\min z MM2}$) for the reactants^{11,12} & products are shown in table (3) and table (4) respectively.

In a strong basic medium two anions from menthone can be obtained, anion Men1 and anion Men2 (scheme 1). The heat of formation of anion (Men. 1) is (-82.905 Kcal/mole), while that for anion (Men. 2) is (-88.936 Kcal/mole). The anion (Men. 1) is less stable than anion (Men. 2), but due to the steric hindrance, attack of the anion (Men. 1) is more probable than the attack of the anion (Men. 2). Moreover, theoretically, the products obtained from reaction of anion (Men. 1) with the cross conjugated ketone are more stable than the products obtained from the reaction of the cross conjugated ketones with anion (Men. 2). This can be observed when the H.F values are compared for all the possible reactions of the two anions (Scheme 1) (Table 4).

Inspection of scheme 1 and table (4) shows that the theoretical parameters H.F, $S.E_{\min 2 AM1}$ and $S.E_{\min 2 MM2}$ for the products do not give a clear distinction between the stability of addition products of route A or route (B) i.e their values are very close. However the physical parameters which were calculated for the reactants^{11,12} (table 3) clarified which route is preferable. The atomic steric energy (A.S.E) values and the extended Huckel charge (E.H.C) for C_4 and C_4' of the central chain of the dienone [1-3] indicate that C_4' is more liable to nucleophilic attack than C_4 . On the other hand C_4 of the dienone, trienone & tetraenone [4-10] is the preferred site for the nucleophilic attack than C_4, C_6 or C_6' .

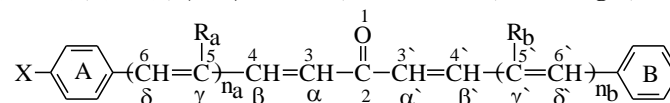
These data indicate that the effect of ring substituent whether e-withdrawing (p-Cl [2],[6]) or e-donating (p-CH₃ [3],[7]) on the addition of Men1 is weak. This unexpected behavior can be attributed to the non-planarity of the phenyl ring (A) with the enone chain which is supported by the values of the dihedral angle for all the reactants (Table 3) and 3D structure^{11,12}. The data obtained from the minimized geometry for compounds [11-20] indicate that these final products are not planar. As a representative model the 3D structure of compound [20] is selected Fig(1). The dihedral angle $\phi_A = + 66.6$ and $\phi_B = + 12.8$ which indicates its non-planarity. The dihedral angle between menthone molecule and the central system is -48.4 which means that the menthone ring is not the same plane with the starting material.


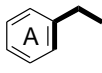
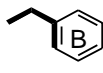

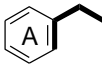
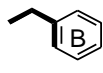

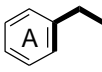
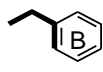

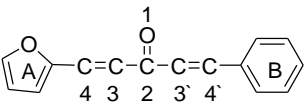
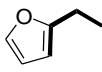
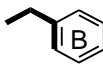

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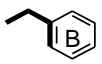
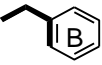
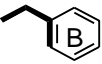
Scheme (1): The suggested mechanism for the reaction of menthone with tetraenone [10]

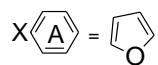
Table(3): THE PHYSICAL PARAMETERS (E.H.C) ; (A.E.D.) ; (H.F.) ; (S.E.)_{Mini AM1} ; [S.E.]_{Mini MM2} ; bond length; Dihedral Angle; (A.S.E.)} FOR COMPOUNDS [1-10]



Comd .No.	X	n _a	n _b	R _a	R _b	CHARGE (Wang-Ford), Extended Hückel charge		BOND LENGTH (Å)		H.F (S.E.) [S.E.] kcal/mole	DIHEDRAL ANGLE (DEGREES)		CHARGE (Wang-Ford), Extended Hückel charge	A.S.E. kcal/mole	
						Atom electron density(A.E.D)		ring A	ring B						
1	H	0	0	-	-	C3	C4			C3=C4 1.34345		C3'=C4' 1.34333	45.227 (-1.451) [-2.899]	 + 4.1	 - 5.3
						(-0.095)	+0.052	(-0.313)	(+0.284)						
						4.2372	4.0373	C=O 1.24260		(-0.520)	(+0.400)				
						C3'	C4'			(-0.236)	(-0.037)				
						(-0.095)	+0.052			4.2370	4.0376				
2	Cl	0	0	-	-	C3	C4	C3=C4 1.34319	C3'=C4' 1.34371	38.264 (-0.912) [-2.526]	 + 11.4	 - 3.2	(-0.230)	(-0.042)	C4=-2.9224 C4'=-2.5613
						(-0.132)	+0.057						(-0.311)	(+0.283)	
						4.2306	4.0429	C=O 1.24247					0.594	+0.389	
						C3'	C4'						(-0.239)	(-0.034)	
						(-0.090)	+0.059						4.2395	4.0340	
3	CH ₃	0	0	-	-	C3	C4	C3=C4 1.34359	C3'=C4' 1.34345	37.474 (-1.350) [-3.035]	 + 12.8	 - 3.3	(-0.239)	(-0.034)	C4=-3.018 C4'=-2.722
						(-0.101)	+0.063						(-0.314)	(+0.284)	
						4.2395	4.0348	C=O 1.24271					(-0.576)	(+0.397)	
						C3'	C4'						(-0.236)	(-0.038)	
						(-0.091)	+0.065						4.2367	4.0469	
4		0	0	-	-	C3	C4	C3=C4 1.34368	C3'=C4' 1.34401	27.084 (15.55) [8.808]	 - 4.2	 + 14.5	(-0.229)	(-0.016)	C4= 0.885 C4'=-1.3651
						(-0.099)	+0.071						(-0.312)	(+0.283)	
						4.2291	4.0166	C=O 1.24266					(-0.520)	(+0.407)	
						C3'	C4'						(-0.238)	(-0.035)	
						(-0.095)	+0.056						4.2384	4.0350	

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						C3	C4	C5	C6	C3=C4	C5=C6								
5	H	0	1	-	H	(-0.236)	(-0.043)			1.34330	C3=C6 ⁺	58.264 (-3.912) [5.753]			-7.4	+7.0	(-0.314) (+0.281)	C4=-0.2332 C4'=-0.6972 C6'=-1.8474	
						-0.090	+0.068			C3'=C4'	1.34557								
						4.2368	4.0379												
						C3 ⁻	C4 ⁻	C5 ⁻	C6 ⁻	C=O									
						(-0.236)	(-0.048)	(-0.155)	(-0.082)	1.24279									
6	Cl	0	1	-	H	(-0.230)	(-0.043)			1.34330	C5'=C6 ⁻	51.269 (-3.363) [5.316]			+15.4	-4.5	(-0.311) (+0.283)	C4=-0.3014 C4'=-0.9337 C6'=-2.0810	
						-0.129	+0.062			C3'=C4'	1.34565								
						4.2303	4.0433												
						C3 ⁻	C4 ⁻	C5 ⁻	C6 ⁻	C=O									
						(-0.238)	(-0.045)	(-0.157)	(-0.080)	1.24262									
7	CH ₃	0	1	-	H	(-0.239)	(-0.035)			1.34365	C5'=C6 ⁻	50.466 (-3.789) [5.830]			+14.6	-3.9	(-0.316) (+0.283)	C4=-0.3310 C4'=-0.9752 C6'=-2.1540	
						-0.099	+0.062			C3'=C4'	1.34556								
						4.2393	4.0354												
						C3 ⁻	C4 ⁻	C5 ⁻	C6 ⁻	C=O									
						(-0.235)	(-0.049)	(-0.154)	(-0.083)	1.24284									
8	H	1	1	H	H	(-0.235)	(-0.049)	(-0.154)	(-0.083)	1.34475	C5=C6	71.252 (-6.832) [8.490]			-9.2	+12.6	(-0.313) (+0.282)	C4=-0.608 C6=-9.057 C4'=-0.814 C6'=-1.008	
						-0.086	+0.062	-0.036	+0.015	C3'=C4'	1.34555								
						4.2357	4.0492	4.1547	4.0832										
						C3 ⁻	C4 ⁻	C5 ⁻	C6 ⁻	C=O									
						(-0.235)	(-0.049)	(-0.154)	(-0.083)	1.24292									
9	H	1	1	CH ₃	CH ₃	(-0.237)	(-0.047)	(-0.087)	(-0.097)	1.34340	C5=C6	62.157 (6.337) [2.166]			+40.0	+46.4	(-0.314) (+0.280)	C4=1.238 C6=-3.924 C4'=-0.767 C6'=-3.966	
						-0.104	+0.056	+0.050	-0.021	C3'=C4'	1.35021								
						4.2375	4.0473	4.0870	4.0974	C5'=C6'	1.35014								
						C3 ⁻	C4 ⁻	C5 ⁻	C6 ⁻	C=O									
						(-0.237)	(-0.047)	(-0.086)	(-0.097)	1.24272									
10	H	1	1	CH ₃	H	(-0.237)	(-0.047)	(-0.086)	(-0.097)	1.34339	C5=C6	66.698 (0.127) [3.153]			+43.1	+5.6	(-0.314) (+0.283)	C4= 1.4251 C6=-4.3136 C4'=-0.4714 C6'=-1.1479	
						-0.105	+0.062	+0.051	-0.020	C3'=C4'	1.35018								
						4.2374	4.0472	4.0869	4.0973	C5'=C6'	1.34556								
						C3 ⁻	C4 ⁻	C5 ⁻	C6 ⁻	C=O									
						(-0.235)	(-0.049)	(-0.154)	(-0.083)	1.24287									

Prod. No.	X	n _a	n _b	R _a	R _b	H.F (kcal/mole)									
						S.E Mini AMI (kcal/mole)									
						anion Men1					anion Men2				
M1A _{1,6} Men1	M1A _{1,4} Men1	Claisen1 Men1	M1B _{1,4'} Men1	M1B _{1,6'} Men1	M1A _{1,6} Men2	M1A _{1,4} Men2	Claisen1 Men2	M1B _{1,4'} Men2	M1B _{1,6'} Men2						
11	H	0	0	---	---	-----	-42.554 26.523 [18.970]	-33.185 20.786 [10.518]	-42.701 24.965 [18.362]	-----	-----	-36.047 35.249 [27.854]	-20.461 31.035 [21.634]	-36.311 35.291 [28.544]	-----
12	Cl	0	0	---	---	-----	-48.850 29.970 [19.293]	-40.382 21.226 [11.024]	-50.189 28.060 [18.650]	-----	-----	-43.604 35.575 [29.338]	-31.643 31.977 [22.570]	-44.256 38.764 [26.193]	-----
13	CH ₃	0	0	---	---	-----	-49.428 33.598 [20.666]	-40.885 20.883 [11.587]	-51.077 29.590 [20.235]	-----	-----	-43.963 35.017 [30.257]	-32.173 31.464 [23.764]	-44.208 38.279 [29.357]	-----
14	X 	0	0	---	---	-----	-62.041 44.748 [28.950]	-49.657 39.904 [12.357]	-59.889 42.059 [31.858]	-----	-----	-57.416 51.097 [39.574]	-45.235 39.904 [33.210]	-56.663 49.972 [42.887]	-----
15	H	0	1	---	H	-----	-34.319 27.118 [16.111]	-20.256 18.448 [8.048]	-33.117 25.087 [18.804]	-27.945 34.455 [25.637]	-----	-29.744 25.354 [22.704]	-19.573 16.354 [19.300]	-28.311 28.271 [22.074]	-18.854 38.241 [27.558]
16	Cl	0	1	---	H	-----	-39.726 27.567 [16.010]	-27.425 18.862 [8.634]	-40.134 26.075 [17.121]	-35.058 33.369 [26.172]	-----	-34.256 24.665 [25.447]	-17.465 19.354 [24.175]	-33.550 23.584 [25.376]	-16.450 26.885 [28.667]
17	CH ₃	0	1	---	H	-----	-37.953 25.169 [16.245]	-26.964 19.331 [8.995]	-37.001 25.421 [17.631]	-30.671 34.259 [25.391]	-----	-34.999 31.548 [25.991]	-18.322 18.450 [22.746]	-34.482 30.369 [26.508]	-20.984 28.357 [30.080]
18	H	1	1	H	H	-14.983 34.034 [26.874]	-18.867 25.630 [15.952]	-5.229 16.933 [5.280]	-18.047 25.564 [16352]	-15.568 34.540 [25.668]	-11.681 36.864 [27.926]	-12.433 28.902 [17.334]	-2.357 18.681 [16.776]	-12.258 28.741 [17.117]	-11.842 36.347 [26.456]
19	H	1	1	CH ₃	CH ₃	-14.770 49.067 [20.198]	-25.723 37.489 [24.553]	-16.251 28.192 [15.542]	-25.854 37.996 [25.173]	-14.207 49.854 [20.176]	-9.357 52.367 [28.247]	-21.951 41.158 [22.611]	-10.248 36.981 [26.547]	-21.042 41.651 [22.324]	-9.657 52.441 [25.247]
20	H	1	1	CH ₃	H	-10.250 42.764 [21.058]	-24.553 29.933 [20.716]	-11.697 22.023 [10.208]	-22.014 29.648 [21.367]	-20.422 35.011 [30.276]	-6.333 43.289 [27.054]	-20.022 32.020 [19.654]	-8.034 29.920 [21.871]	-20.226 28.648 [20.091]	-14.325 42.092 [33.226]

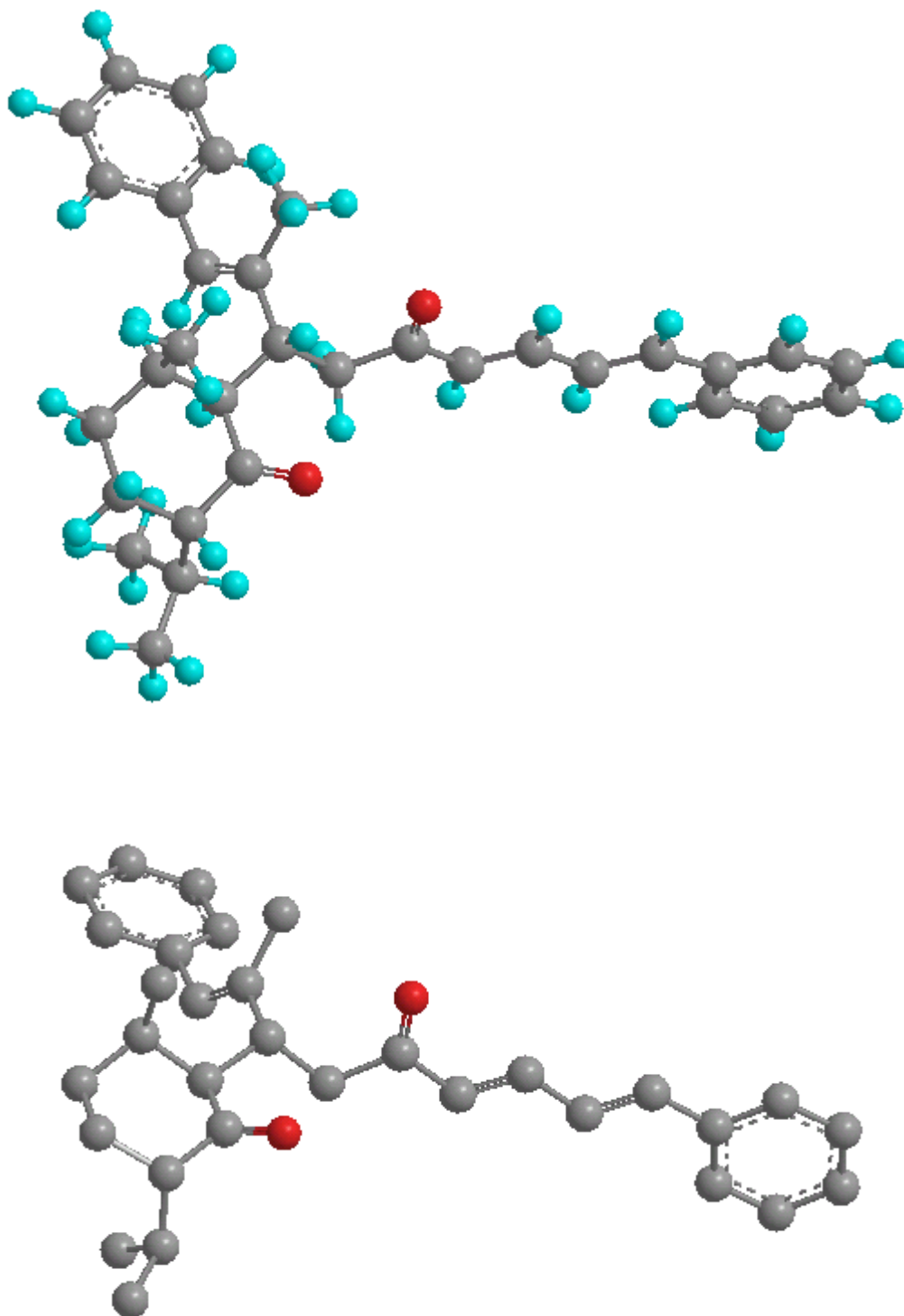


Figure (1): The 3D-structures of compound [20]

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