

Synthesis and Spectral Characterization of some Fused Pyrimidine Thiones

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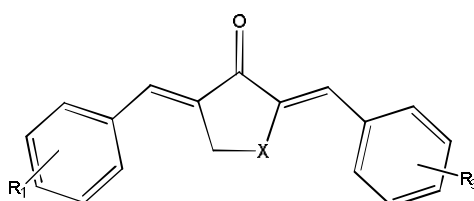
Abstract

The 2,6-diarylidene cyclohexanones had been synthesized by the reaction of Claisen-Schmidt between cyclohexanone and different substituents of para benzaldehydes. The prepared 2,6-diarylidene cyclohexanones were condensed with thiourea under basic conditions (sodium ethoxide in ethanol) to produce pyrimidine thiones "Thiopyrimidines"(8-14). The structures of the reactants (2,6-diarylidene cyclohexanone) and the products (pyrimidine thiones) were suggested in the light of spectral analyses (UV, IR, ¹H-NMR, ¹³C-NMR, and HPLC-Mass). The mechanism of the product formation was suggested according to the data information using ChemDraw ultra 12.0.

Keyword: 2,6-diarylidene cyclohexanone, pyrimidine thiones, Claisen-Schmidt reaction.

Introduction:

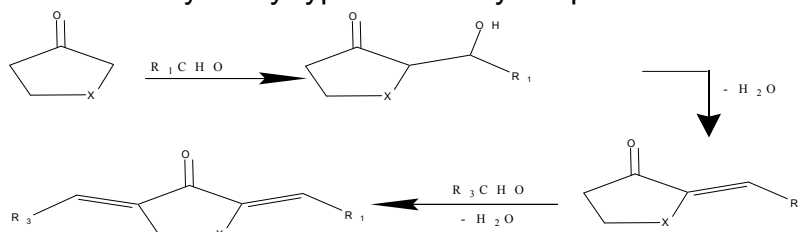
The bis-arylidene cycloalkanone compounds or benzyldenone cycloalkanone are very important building units for many heterocyclic systems having biological activities like dihydropyrazole and substituted pyridine or derivatives (Tyndall, et al., 1988) (JF, 2003), and the system contain the cyclic pyrrole and Pyrazoline or isooxazoline (Venkatapuram, et al., 2004), these compounds were used to prepare many biologically active pyrimidine derivatives (Deli, et al., 1984), which can be changed to new compounds by reactions (Luke, et al., 2004).



$R_1 = R_3$ Symmetrical ; $R_1 \neq R_3$ Unsymmetrical

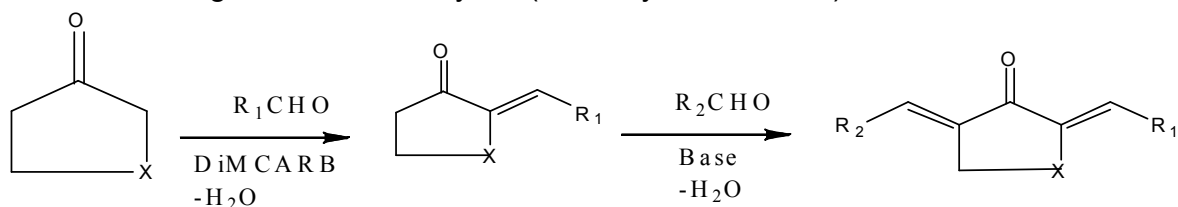
$X = \text{CH}_2, (-\text{CH}_2-)_2, (-\text{CH}_2-)_3$

The prepared α, β - unsaturated ketone using Claisen-Schmidt reaction of aldehyde and cyclic ketone depends on the nature of the product and number of moles of reactant, that means, the synthesis of unsymmetrical bis-arylidene alkanone using aldol condensation by many types of aldehydes proceeds as follows:



$X = \text{CH}_2, (-\text{CH}_2-)_2, (-\text{CH}_2-)_3$

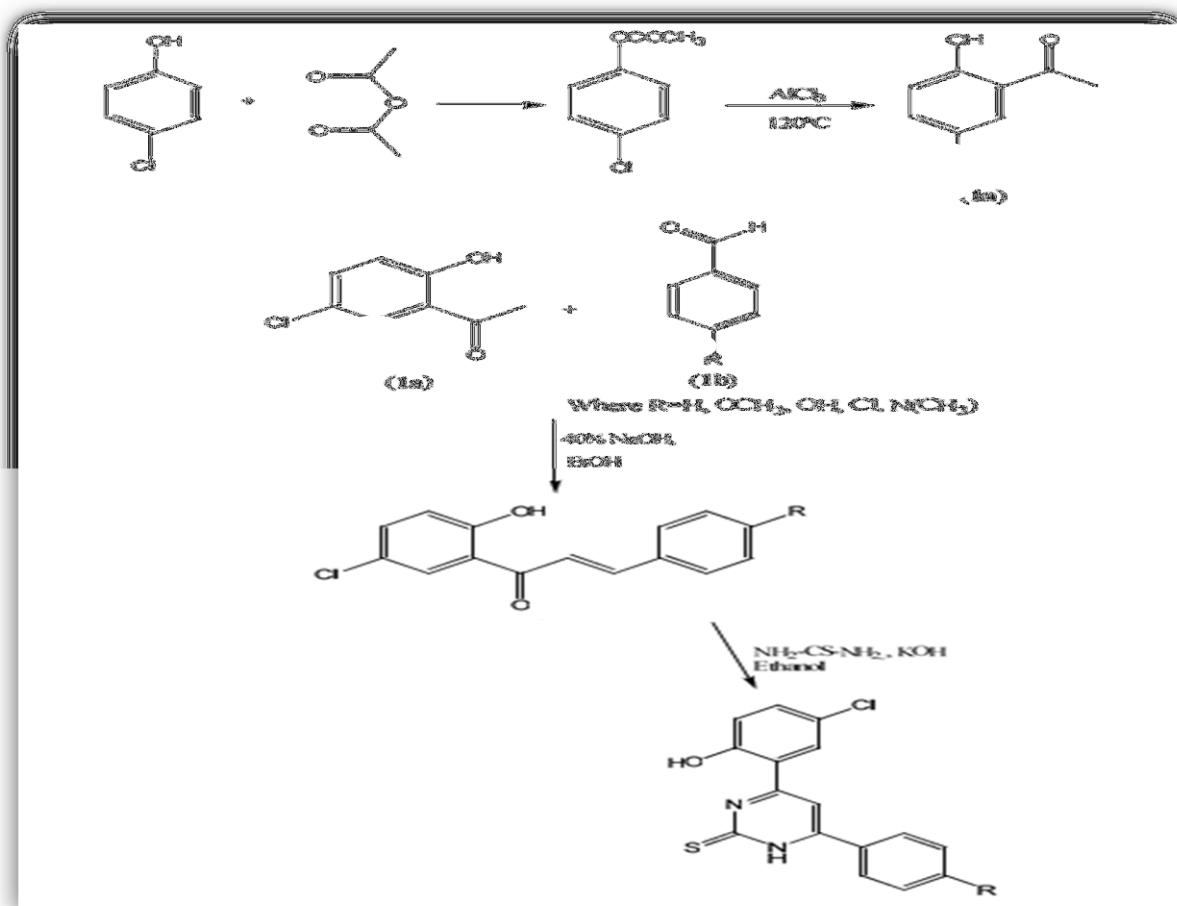
On the other hand, synthesis of symmetrical bis-arylidene alkanone can be carried out using the same aldehydes (Anthony, et al., 2007).



DiMCARB = Dimethyl ammonium dimethyl caramate

$X = -\text{CH}_2-, (-\text{CH}_2\text{CH}_2-)$

The reaction between ethyl cyanoacetate, thiourea and the appropriate aldehydes, namely, 3-methoxy benzaldehyde, 2,5-dimethoxy-benzaldehyde and dimethoxy benzaldehyde produce new pyrimidine thiones derivatives (Ahmad, et al., 2014). A new study for the synthesis of pyrimidine derivatives (1-(4-aryl-6-methyl-2-thioxo-1, 2, 3, 4-tetrahydropyrimidine-5-yl)-ethanone) was obtained from the reaction of thiourea with acetylacetone and aromatic aldehydes and utilized for synthesis of a number of pyrimidine thione derivatives (Mosaad, et al., 2012). Another investigation was the synthesis and characterization of some new 3,5-disubstituted pyrimidine and pyrimidine thione derivatives start from 2-chlorophenol through multi-step reaction with different aryl aldehyde in 40% NaOH, followed by cyclization process with thiourea to give the final product (Dhote, 2013)



Experimental

All melting points were recorded using capillary melting points instrument (BUCHI Melting Point B-540). IR spectra (KBr , $\nu \text{ cm}^{-1}$) were measured on SHIMADZU (FT-IR) spectrophotometer. UV spectra were delivered by Agilent Cary-100 (UV-Visible Spectrophotometer). $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra were displayed on BRUKER 300-MHz spectrometer (Iran) using DMSO as a solvent and the 2,6-diarylidene cyclohexanone were identified by (Water HPLC) to give a mass calculated and UV-visible as an output detector.

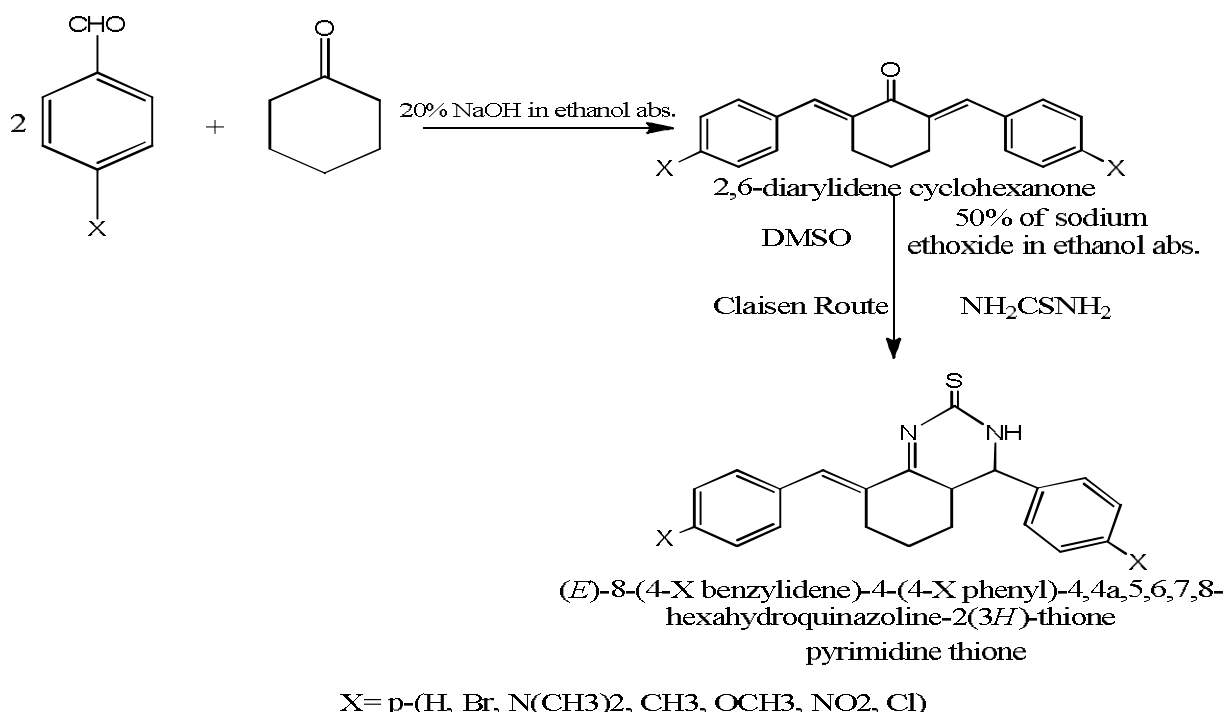
1- Synthesis of [1- 2,6-diarylidene cyclohexanone 7]:

Seven compounds of 2,6 bis-diarylidene cyclohexanone (compounds 1-7) have been synthesized as recorded in Table (1). A solution of (2.0g, 5×10^{-5} mmole) sodium hydroxide in (10ml, 0.171×10^{-3} mmole) absolute ethanol is placed in (50ml) round bottomed flask containing (15ml, 0.256×10^{-3} mmole) absolute ethanol and (7.5 mmole) cyclohexanone provided by mechanical stirrer. Stirring is then started and (15 mmole) of pure benzaldehyde (or its substituents) is added step by step. The heat is kept at room temperature while the pH is kept constant at 12. Vigorous stirring is continued for about 3hrs. until the medium turns very thick. The product is filtered then washed twice with absolute

ethanol and dried, the solid is then recrystallized from ethanol or acetone to get a yellowish pure product.

2- Synthesis of fused pyrimidine thione [8-14]:

Seven compounds of pyrimidine thione [8-14] were synthesized as follows: Two solutions were prepared, the first contained (0.23g, 3 mmole) thiourea dissolved in 0.5 ml 1:1 sodium ethoxide / absolute ethanol solvent, the other contained (0.27g, 1×10^{-3} mmole) of compound (1) dissolved in (5ml) dimethyl sulfoxide (DMSO). The two solutions were mixed together in round bottomed flask (50ml), refluxed at 80°C on a water bath for about 12hrs with stirring. Then cooled and poured in ice cold water. The product was separated, washed twice with cold distilled water to get rid of the base and recrystallized from ethanol (Scheme-1).



Scheme - 1

Results and Discussion

The current work is concerned with the syntheses of fused pyrimidine thione containing different groups as substituents at the para position. Compounds [1-7] were synthesized by the reaction of thiourea with 2,6-diarylidene cyclohexanone, via Claisen-Schmidt reaction, from aromatic aldehydes and cyclohexanone in basic medium (Scheme-1).

Formation of the intermediates 2,6-diarylidene cyclohexanone [1-7] was confirmed on the basis of their IR, UV-visible spectrophotometer, HPLC-MS data, and $^1\text{H-NMR}$, $^{13}\text{C-NMR}$. The series of 2,6-diarylidene cyclohexanone [1-7] exhibit different substituents. The IR spectrum for the compound (1) showed strong

band at 1689cm^{-1} which was corresponded to the C=O stretching vibration, while the 1602cm^{-1} band was related to C=C group, and the $\text{C}=\text{C}$ stretching vibration appeared near 1489cm^{-1} (Jihad, 2011) as shown in table (2).

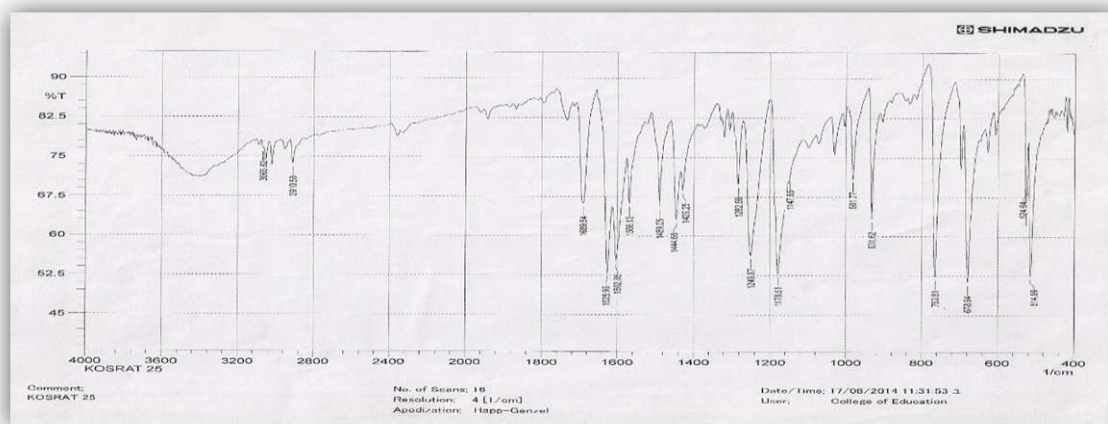


Figure (1): IR spectrum for compound (1)

The UV absorption spectrum was shown in $\lambda_{\text{max}}=344\text{nm}$ in ethanol solvent, as shown in the table (2)

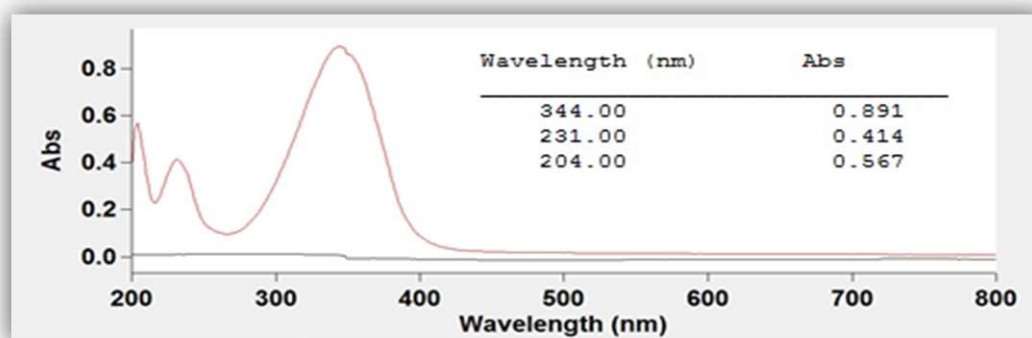


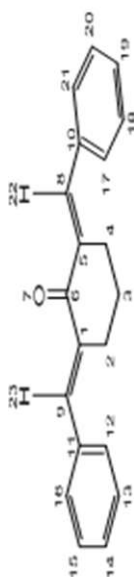
Figure (2): UV-Visible spectrophotometer spectrum for compound (1)

The HPLC-MS showed a peak at 275.14 by using ES+ technique as shown in table (2). The $^1\text{H-NMR}$ showed a triple signal at $\delta 2.869\text{ppm}$ for the four protons of the cyclohexanone next to double bond (H2, H4), while (H3) showed pentet signal due to the two protons at $\delta 1.682\text{ppm}$, (H8, H9) showed a singlet signal for the two olefinic protons at $\delta 7.630\text{ppm}$, and the (Ar-H) showed multiplet signal for the five aromatic protons between $\delta 7.354\text{--}7.531\text{ppm}$ as shown in Table (3).

The $^{13}\text{C-NMR}$ spectrum showed the variable peak which is attributed to the following carbons: (C2, C4) at $\delta 28.297\text{ppm}$, (C3) at $\delta 22.860\text{ppm}$, (C1, C5) at $\delta 127.911\text{ppm}$, (C6) at $\delta 189.384\text{ppm}$, (C8, C9) at $\delta 136.384\text{ppm}$, and (Ar-C) at $\delta 135.557\text{ppm}$. as shown in Table (4).

For the compound (2) which has (-Br) substituted on the benzene ring reflects a (C-Br) stretching vibration band in IR spectrum at 519cm^{-1} , and the remaining bands were similar to that of the compound (1). UV spectrum was shifted to the 334.00nm . Mass spectrum showed a high line at 433.03 which is related to compound (2), $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ are similar to compound (1), except the

splitting of Ar-H which seemed as dd (doublet of doublet). For compound (3) with (-N(CH₃)₂) group substituted on the benzene ring, showed C-N band at 1180cm⁻¹ in IR spectrum, while the remaining bands seemed to be similar to compound (1). UV spectrum showed λ_{\max} at 448.00nm. Mass spectrum showed a high peak at 361.27 which is related to compound (2) using the same technique as for compound (1), H¹-NMR showed a singlet signal for the (-N(CH₃)₂) at 3.329 ppm related to the six protons as a singlet band, and all other signals are similar to those of compound (1), C¹³-NMR exist at 40.775 ppm which is attributed to (-CH₃) groups for the dimethyl amino group. For the compound (4) with a (-CH₃) substituent on the benzene ring showed stretching vibration of (C-C) bond the in IR at 986cm⁻¹, all other bands are similar to compound (1), UV showed λ_{\max} at 341.00nm, Mass spectrum has a high peak value at 303.18 which is related to compound (4). For the compound (5) with (-OCH₃) group on the benzene ring, showed(C-O-C) stretching vibration band at 2843cm⁻¹ in IR spectrum, and the remaining bands were similar to compound (1), UV spectrum λ_{\max} at 364.00nm, Mass spectrum showed a high peak at 335.00 which prove the molar mass of compound (5) using the same technique for the compound (1), H¹-NMR showed the signal for the (-OCH₃) at 3.778ppm(six proton) as singlet signal, while all other bands are similar to compound (1), C¹³-NMR showed at line 57.459ppm which is attributed to the para (-OCH₃) group substituent at the benzene ring, and all other bands were similar to compound (1). For the compound (6) with para (-NO₂) group at the benzene ring, showed the IR stretching vibration for (C-NO₂) at 1343cm⁻¹, while the remaining bands were similar to the compound (1), UV spectrum showed λ_{\max} at 337.00nm, Mass spectrum showed a high peak at 365.18 which is related to compound (6) using the same technique as for the compound (1), H¹-NMR and C¹³-NMR were also similar to the compound (1). No any peak for the (C-NO₂) bond was displayed using this technique, but only the Ar-H seemed as (dd) due to the para substitution. Finally, for the compound (7) with para (-Cl) on the benzene ring showed (C-Cl) band stretching vibration IR spectrum at 799cm⁻¹, and the remaining bands were also similar to the compound (1). UV spectrum was shifted to the λ_{\max} 333.00nm, Mass spectrum showed a high band at 345.08ppm. All the information are tabulated in the Table 2, 3, and 4 (Paris, and Thomas , 2006) (Pretsch, et al., 2009).

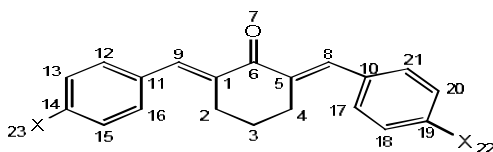


TABLE(1):- PHYSICAL AND SPECTRAL DATA OF THE 2,6-DIARYLIDENECYCLOHEXANONE[1-7].

Compound No.	Structures	Name of structures	Reaction time (hrs.)	Colors	m.p. °C	Yield %
1		2,6-diphenylidene cyclohexanone	3	Yellow	120-122	41
2		2,6-bis(4-bromophenylidene) cyclohexanone	3	Deep Yellow	165-167	60
3		2,6-bis(4-(dimethylamino)phenylidene) cyclohexanone	3	Orange	240-242	40
4		2,6-bis(4-methylphenylidene) cyclohexanone	3	Yellow	165-168	60
5		2,6-bis(4-methoxyphenylidene) cyclohexanone	3	Deep Yellow	214-216	55
6		2,6-bis(4-nitrophenylidene) cyclohexanone	3	Brown	200-201	31
7		2,6-bis(4-chlorophenylidene) cyclohexanone	3	Yellow	140-141	50

Table (2): IR, HPLC-Ms, and UV-Visible spectrophotometer for compounds [1-7]

Compu nds No.	I.R. (KBr), ν (cm^{-1})										LC - Mass		UV (Ethanol abs.) λ_{max} (nm)
	C=C	C-N	C=C	C=O	C-O-C	C-Cl	C-Br	C-NO ₂	C-C	M.Wt Calc.	M.Wt ES+		
1	1489	-----	1602	1689	-----	-----	-----	-----	-----	274.4	275.14	344	
2	1487	-----	1606	1693	-----	519	-----	-----	-----	432.1	433.03	334	
3	1521	1180	1599	1672	-----	-----	-----	-----	-----	360.5	361.27	448	
4	1510	-----	1603	1688	-----	-----	-----	986	-----	302.4	303.18	341	
5	1510	-----	1616	1697	2843	-----	-----	-----	-----	334.4	335.00	364	
6	1516	-----	1589	1668	-----	-----	1343	-----	-----	364.4	365.18	337	
7	1489	-----	1575	1667	-----	799	-----	-----	-----	343.2	345.08	333	

Table (3): ¹H-NMR for compounds 1, 2, 3, 5, 6

Compounds No.	¹ H-NMR (DMSO),ppm				
	H2, H4	H3	H8, H9	Ar-H	Others
1	2.869 4H, t	1.682 2H, p	7.630 2H, s	7.354-7.531 5H, m	
2	2.825 4H, t	1.679 2H, p	7.602 2H, s	7.466-7.543 5H, m	
3	2.852 4H, t	1.706 2H, p	6.765 2H, s	7.318-7.687 5H, m	3.329 6H,s
5	2.845 4H, t	1.684 2H, p	6.983 2H, s	7.481-7.560 5H, m	3.778 6H,s
6	3.059 4H, t	1.718 2H, p	7.654 2H, s	8.169 5H, m	

Table (4): ¹³C-NMR for compounds 1, 2, 3, 5, 6

Compound No.	¹³ C-NMR (DMSO),ppm							
	C2, C4	C3	C1,C5	C6	C8,C9	Ar-C	Ar-C-X	Others
1	28.297	22.860	127.91 1	189.38 4	136.84 5	135.55 7	-----	
2	28.138	22.725	131.30 6	189.58 0	137.37 0	135.59 2	122.73 5	
3	28.331	22.525	132.07 2	190.34 0	136.36 4	134.21 2	150.14 1	40.775 (-CH ₃)
5	28.139	22.041	131.60 4	189.44 9	136.49 9	134.59 8	160.30 7	57.459 (-OCH ₃)
6	28.012	21.813	124.75 4	189.34 2	135.32 5	131.31 3	147.32 1	

For the series of the products [8-14], the identification is based on the spectral analysis which are (IR, UV-Visible, and (¹H, ¹³C)-NMR). For the parent compound (8) (no substitution on benzene ring), the IR spectrum showed a band at 1188cm⁻¹

corresponding to the $\nu(\text{C}=\text{S})$ stretching, and a band at 3199cm^{-1} related to (N-H) group, while a (C=C) stretching vibration appeared near 1601cm^{-1} , (C=N) appeared at 1623cm^{-1} , (C-N) at 1028cm^{-1} , and finally 1539cm^{-1} is attributed to the stretching of the aromatic ring ($\text{C}=\text{C}$) as shown in Table (6). The UV absorption spectrum showed $\lambda_{\text{max}}=263\text{nm}$ in DMSO solvent, as shown in the Table (6), which means the occurrence of a hypsochromic shift (blue shift) compared to the reactant $\lambda_{\text{max}}=344\text{nm}$, which may be attributed to the disappearance of conjugation.

The $^1\text{H-NMR}$ showed a multiplet signal at 2.800ppm for the three protons of the (H2, H22), while (H3, H4) displayed a multiplet signal for the four proton at 1.629ppm, (H5) showed a quartet signal for one proton at 2.267ppm. The (H9) showed a singlet signal for one proton at 3.562, and the (Ar-H) showed multiplet signal for the five protons at 7.519 ppm as shown in Table (7).

The $^{13}\text{C-NMR}$ spectrum showed the variable peak which is attributed to the following carbons: (C1) at 128.160 ppm, (C2) at 27.325 ppm, (C3, C4) at 25.011 ppm, (C5) at 39.115 ppm, (C6) at the 167.373 ppm, (C8) at 58.287 ppm, (C9) at 129.271 ppm, (C23) at 183.970 ppm, and (Ar-C) at 137.362ppm. this compound has unsubstituted benzene ring, as shown in Table (8).

For the compound (9) with p(-Br) on the benzene ring showed stretching vibration for (C-Br) bond in IR spectrum at 625cm^{-1} , and the remaining bands were similar to as in compound (8). UV spectrum showed λ_{max} shifted to the 264.00nm (blue shift). $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ were at similar position as compared to compound (8) i.e. not displayed any peak for the C-Br bond. For compound (10) with p(-N(CH₃)₂) group showed (-N-C-) band in IR spectrum at 1056cm^{-1} , and the remaining bands were similar to compound (8). UV spectrum was shifted to the 400.00nm (Bathochromic shift (i.e. red shift)) This high value of λ_{max} may be attributed to the lone pair of the nitrogen atom. For compound (11) with p(-CH₃) substituent showed (C-C) band in IR spectrum at 951cm^{-1} , and the remaining bands were similar to compound (8). UV spectrum was shifted to the $\lambda_{\text{max}}= 269.00\text{nm}$. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ were similar to compound (8), showed the signal at $\delta(2.350\text{ppm})$ as a singlet for the six protons of (Ar-CH₃), while for the $^{13}\text{C-NMR}$ showed the peak at 21.367ppm which is attributed to the (-CH₃) group. For compound (12) with p(-OCH₃) showed (C-O-C) band in the IR spectrum at 2835cm^{-1} , and the remaining bands were similar to compound (8). UV spectrum was shifted to $\lambda_{\text{max}}= 284.00\text{nm}$. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ were similar to compound (8), showed a signal at $\delta(3.778\text{ppm})$ as a singlet for the six protons of (Ar-CH₃) in $^1\text{H-NMR}$, while for the $^{13}\text{C-NMR}$ showed the peak at $\delta(54.905\text{ppm})$ which was attributed to the (-OCH₃) group. For compound (13) p(-NO₂) showed (C-NO₂) band in the IR spectrum at 1344cm^{-1} , and the remaining bands were similar to compound (8). UV spectrum was shifted to

λ_{\max} =272.00nm. H^1 -NMR and C^{13} -NMR were similar to compound (8). For the compound (13) with p(-Cl) showed (C-Cl) band in the IR spectrum at $6797cm^{-1}$, and the remaining bands were similar to compound (8). UV spectrum was shifted to λ_{\max} = 263.00nm. All information was tabulated in Table 6, 7, and 8 for the above mentioned compound (Usama, et al., 2010)

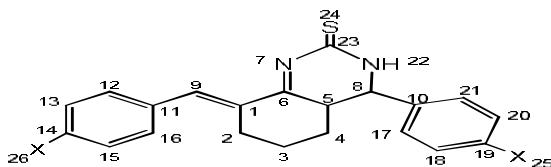


TABLE(5):- PHYSICAL AND SPECTRAL DATA OF THE FUSED PYRIMIDINE THIONES [8-14]:

Compound No.	Structures	Name of structures	Reaction time (hrs.)	Colors	m.p., oC	Yield %
8		8-benzylidene-4-phenyl-4,4a,5,6,7,8-hexahydroquinazoline-2(3H)-thione	12	Brown-Yellow	130-132	45
9		8-(4-bromobenzylidene)-4-(4-bromophenyl)-4,4a,5,6,7,8-hexahydroquinazoline-2(3H)-thione	12	Brown-Yellow	140-141	40
10		8-(4-(dimethylamino)benzylidene)-4-(4-(dimethylamino)phenyl)-4,4a,5,6,7,8-hexahydroquinazoline-2(3H)-thione	12	Brown-Yellow deep	129	45
11		8-(4-methylbenzylidene)-4-(p-tolyl)-4,4a,5,6,7,8-hexahydroquinazoline-2(3H)-thione	12	Brown-Yellow	132	50
12		8-(4-methoxybenzylidene)-4-(4-methoxyphenyl)-4,4a,5,6,7,8-hexahydroquinazoline-2(3H)-thione	12	Deep Yellow	80-83	50
13		8-(4-nitrobenzylidene)-4-(4-nitrophenyl)-4,4a,5,6,7,8-hexahydroquinazoline-2(3H)-thione	12	Brown-Yellow	156-157	30
14		8-(4-chlorobenzylidene)-4-(4-chlorophenyl)-4,4a,5,6,7,8-hexahydroquinazoline-2(3H)-thione	12	Deep Brown-Yellow	99-100	50

Table (6): IR, and UV-Visible spectrophotometer for fused pyrimidine thiones compound [8-14]

Compu nds No.	I.R. (KBr), ν (cm^{-1})											UV (DMSO solvent) λ_{max} (nm)
	C=C	C-N	C=N	C=C	N-H	C-O-C	C-Cl	C-Br	C-NO ₂	C-C	C=S	
8	1539	1028	1623	1601	3199	-----	-----	-----	-----	-----	1188	263
9	1528	1071	1678	1589	3393	-----	-----	625	-----	-----	1011	264
10	1522	1056	1659	1605	3312	-----	-----	-----	-----	-----	1028	400
11	1539	1114	1647	1611	3188	-----	-----	-----	-----	951	1018	269
12	1539	1113	1636	1607	3208	2835	-----	-----	-----	-----	1028	284
13	1516	1107	1644	1593	3321	-----	-----	-----	1344	-----	1017	272
14	1541	1015	1684	1595	3314	-----	797	-----	-----	-----	1092	263


 Table (7): ^1H -NMR for compounds 8, 9, 11, 12, 13

Compounds No.	^1H -NMR (DMSO), ppm						
	H2, H22	H3, H4	H5	H8	H9	Ar-H	Others
8	2.800 3H, m	1.629 4H, m	2.267 1H, q	3.562 1H, d	6.476 1H, s	7.519 5H, m	-----
9	2.759 3H, m	1.448 4H, m	2.160 1H, q	3.294 1H, d	6.318 1H, s	7.606 5H, m	-----
11	2.800 3H, m	1.529 4H, m	2.267 1H, q	3.362 1H, d	6.476 1H, s	7.519 5H, m	Ar-CH ₃ (2.350) 6H,s
12	2.753 3H, m	1.201 4H, m	2.256 1H, q	3.334 1H, d	6.617 1H, s	7.885 5H, m	Ar-OCH ₃ (3.778) 6H,s
13	3.003 3H, m	1.454 4H, m	2.264 1H, q	4.026 1H, d	6.585 1H, s	7.965 5H, m	-----

 Table (8): ^{13}C -NMR for compounds 8, 9, 11, 12, 13

Compound No.	^{13}C -NMR (DMSO), ppm									
	C1	C2	C3, C4	C5	C6	C8	C9	C23	Ar-C	Ar-C-X
8	128.1 60	27.32 5	25.0 11	39.11 5	167.3 73	58.28 7	129.2 71	183.9 70	137.3 62	---
9	124.3 62	26.85 4	24.0 12	39.15 4	165.0 13	54.22 7	127.4 90	181.0 33	132.5 90	---
11	126.7 37	27.08 5	22.3 86	39.09 8	161.0 23	57.12 7	129.2 52	183.6 14	133.6 44	-CH ₃ 21.36 7
12	127.5 72	28.13 1	23.0 83	39.08 9	160.3 41	59.26 4	129.8 46	188.9 29	132.3 92	- OCH 3 54.90 5
13	126.7 26	27.78 9	22.3 97	39.29 8	161.7 12	58.03 3	129.4 09	183.0 13	133.8 52	---

Acknowledgment:

We offer our affection, appreciation and indebtedness to Koya University-Faculty of Science and Health, namely, Chemistry Department, for their help in the practical part of the research in chemistry laboratories.

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پوخته

لهم تویژینه وهیه دا ناویته کانی 2,6-دای ارایلدینی بازنهیی ناماده کرا به ریگای کلیسن-شمیدت، نهوش به کارلیک کردنی هیکسانونی بازنهیی له گه ل چه ند ناویته یه کی بنزالدیهاید بریخراو له شوینی بارای. وه ههنگای دواي نهو هه نساین به چرکردنه وهی 2,6-دای ارایلدینی بازنهیی ناماده کراو له گه ل ثایویوریا به به کارهینانی ناوه ندیکی تفتی (نیثوکسید السودیوم له ناو نیثانول) بو نه وهی (بریمیدیناتی ثایون) (8-14) مان دهستان بکه ویته. هه موو ناویته ناماده کراوه کان (ناوه ندی و به ره هم هاتوو) ناسرانه وه و شیوگی کیمیاوی جیگیر کرا به به کارهینانی شه به نگه کانی (تیشکی سه روو وه نه وشه یی، تیشکی ژیر سوو، له ره له ری موگناتیسی بو کاربون و هایدروجن، و HPLC-Mass). و میکانیزمی پیشنیازکراو بو نه م ناویتانه نه نجام درا به به کارهینانی زانیاریه ژماره یه کان که له شیکردنه وهی شه به نگی وهرگیرابوو به به کارهینانی به رنامه ی 12.ChemDraw.

الخلاصة

I. تم تحضير المركبات 2,6- داي ارايلدين سايكلووهكسانون بطريقة كليسن - شميدت، وذلك من خلال تفاعل الهكسانون الحلقي مع مختلف المعوضات في موقع البارابنزالديهايد. ويليها تكاثف 2,6- داي ارايلدين سايكلووهكسانون المحضر مع ثايويوريا في الوسط القاعدي (ايثوكسيد الصوديوم في ايثانول المطلق) للحصول على (البريميدينات الثايون) (8-14). جميع المركبات المحضرة (الوسطية و النهائية) شخست وثبتت تراكيبيها بواسطة (الاشعة فوق البنفسجية والاشعة تحت الحمراء والرنين المغناطيسي للهيدروجين والكاربون و كذلك التقنية كروموتوغرافيا السائل العالية الاداء). وتم اقتراح الميكانيكية الحصول على النتائج الوسطية و النهائية من خلال المعلومات الرقمية المستحصلة من التشخيص الطيفي للمركبات وذلك من خلال استخدام برنامج ChemDraw 12.