



Synthesis and characterization of some New Derivatives from 2-Mercaptobenzothiazole

Mohammad R. Ahmad, Athraa H. Ahmad*

Department of Chemistry, College of science, University of Baghdad, Baghdad, Iraq

Abstract

In this work 2- mercaptobenzothiazole (2-MBT) and some of its derivatives(1, 14 ,27) were prepared by using home made Autoclave .The synthesis involve treatment of 2- MBT or some of its derivatives with chloro acetyl chloride to give 1- chloro acetyl -2- MBT or the corresponding derivatives (2,15,28) . the product was treated with phenyl hydrazine to give the phenyl hydrazide derivatives (3,16,29) . The new derivatives(4-13, 17-26,30-39) were synthesized by reaction of the phenyl hydrazide derivatives with different aromatic aldehydes in the presence of Acetic Acid . Structure of all the prepared compounds confirmation were proved using FTIR , elemental analysis (C .H .N .S) in addition to melting points.

Keyword: 2- mercaptobenzothiazole (2-MBT), schiff bases, chloro acetyl-2-MBT, phenyl hydrazide derivative.

تحضير وتشخيص بعض المشتقات الجديدة من 2- مركبتو بنزو ثيازول

محمد رفعت احمد، عذراء حكمت احمد*

قسم الكيمياء، كلية العلوم، جامعة بغداد، بغداد، العراق

الخلاصة:

حضر 2- مركبتو بنزو ثيازول وبعض مشتقاته (1 ، 14 ، 27) و تمت معاملة 2- مركبتو بنزو ثيازول او احد مشتقاته مع كلورو استيل كلورايد ليعطي كلورو استيل 2- مركبتو بنزو ثيازول (2) او المشتقات المقابلة له (15 ، 28). والذي بدوره يتفاعل مع فنييل هيدرازين ليتحول الى مشتقات فنييل هيدرازيد (3 ، 16 ، 29) . تم مفاعلة مشتقات الهيدرازيد مع الالديهيدات الاروماتية المختلفة بوجود حامض الخليك للحصول على مشتقات جديدة (4-13 ، 17-26 ، 30-39) . تم تشخيص المركبات المحضرة بمطياف (FT IR) والتحليل الدقيق للعناصر (C.H.N.S) اضافة الى درجة الانصهار .

Introduction

The chemistry and pharmacology of benzothiazole derivatives have been of great interest because of its various biological activity [1,2]. The benzothiazole has received the attention of medicinal chemists due to their wide range of biological activities which include anti – inflammatory [3] antitumor[4], vasodilator[5], antitubercular[6], antifungal[7], antimicrobial [8] ,anticancer [9], anti diabetic [10] and anti bacterial activities [11]. 2-Mercaptobenzothiazole (MBT) is an important scaffold known to be associated with several biological activities, and its derivatives are manufactured worldwide for a wide variety of applications. S-acetylhydrazide hydrazones [12] and S-acyl [13] derivatives of MBT were reported to possess antifungal and antibacterial activities, 2-MBT is also used in non-biological application , it serve as plant growth regulators[14] and used as accelerators in rubber vulcanization,

*Email: adraa.ahmad@yahoo.com

antioxidants, dyes, polymers and photographic materials [15], stainless steel in aqueous solutions of NaCl [16], steel, copper and alloys in HCl [17], mild steel and Zinc in Phosphoric acid [18,19]. It was also widely used as an accelerator in rubber processing [20], and antioxidant for rubber and plastics [21]. 2-Mercaptobenzothiazole and its derivatives display insecticidal properties [22], it is a well-known analytical reagent for mercury, and mono layers of 2-MBT on gold have been used for the electro analytical determination of Hg (II), Fe (II), Cd(II) [23] and were also found to be useful in the leather industry [24].

Experimental

Chemicals: Starting chemical compounds were obtained from Merck, BDH, Sigma Aldrich and Fluka and used as received.

Instruments

All chemicals used were of high purity as the manufacturers supplied them. The FT-IR spectra in the range (4000-200) cm^{-1} were recorded as KBr disc on a Shimadzu FT-IR 8300 spectrophotometer, elemental analysis (C.H.N.S) was carried out in Ministry of Oil. Melting points were determined using scientific FIC melting point SMPLU-K and were uncorrected. The 2-MBT was prepared using a The manufacturer domestic autoclave made from stainless steel with a capacity of 300 ml and of 12.5 cm diameter. As shown below in figure-1.



Figure 1- The manufacturer domestic Autoclave

Synthesis of 2-MBT and some its derivatives (1, 14, 27). [25]

Aniline or some of its derivatives (0.25 mol) was mixed with (25 ml) Absolute ethanol, (15 ml, 0.25 mol) of carbon disulfide and (8 g, 0.25 mol) sulfur. The mixture was transferred in to Autoclave after closing it very well to get a high temperature and pressure. The set-up was heated in a sand bath at 180 °C for (6-8 hrs). Then the mixture was placed in a beaker and with addition of 7 ml of 10% Sodium hydroxide to get rid from unreacted amine and some concentrated hydrochloric acid until the mixture became acidic solution for precipitation of thiol. The precipitate was filtered off and (7 ml) 25 % sodium carbonate was added. The filtered mixture was dried and recrystallized from ethanol and water. Physical properties and nomenclature of compound (1, 14, 27) are listed in table-1.

Synthesis of chloro acetyl -2- MBT and some its derivatives (2,15,28). [26]

Equimolar solution of 2-MBT or its derivatives (0.1 mol) and chloro acetyl chloride (0.1 mol) in chloroform (30 ml) in the presence of NaOH was refluxed on water-bath for about 12 hr. The solvent was removed by vacuum. The residue was recrystallized from methanol to furnish the product. Physical properties and nomenclature of compounds (2,15,28) are listed in table-1.

Synthesis 1-phenyl hydrazino acetyl -2-MBT and some its derivatives (3,16,29). [27]

Compounds (2,15,28) (2.72 g, 0.009 mol) and phenyl hydrazine (0.9 g, 0.009 mol) in 8 ml ethanol was stirred at room temperature for 2 days. The solid precipitate was filtered off and recrystallized from benzene to give the product according to scheme (1). Physical properties and nomenclature of compound (3,16,29) are listed in table-1.

Synthesis 1-[α -(Arylidine hydrazino) acetyl]-2-MBT and its derivatives (4-13, 17-26, 30-39). [27]

Equimolar quantities of compounds (3,16,29) (0.001 mol,0.347 g) and suitable aromatic aldehydes (0.001 mol) in (25 ml) of ethanol containing few drops of acetic acid was refluxed on water bath for about 5 hrs. The solvent was removed under reduced pressure to offer the product . Physical properties and nomenclature of compounds (4-13, 17-26,30-39) are listed in table-1.

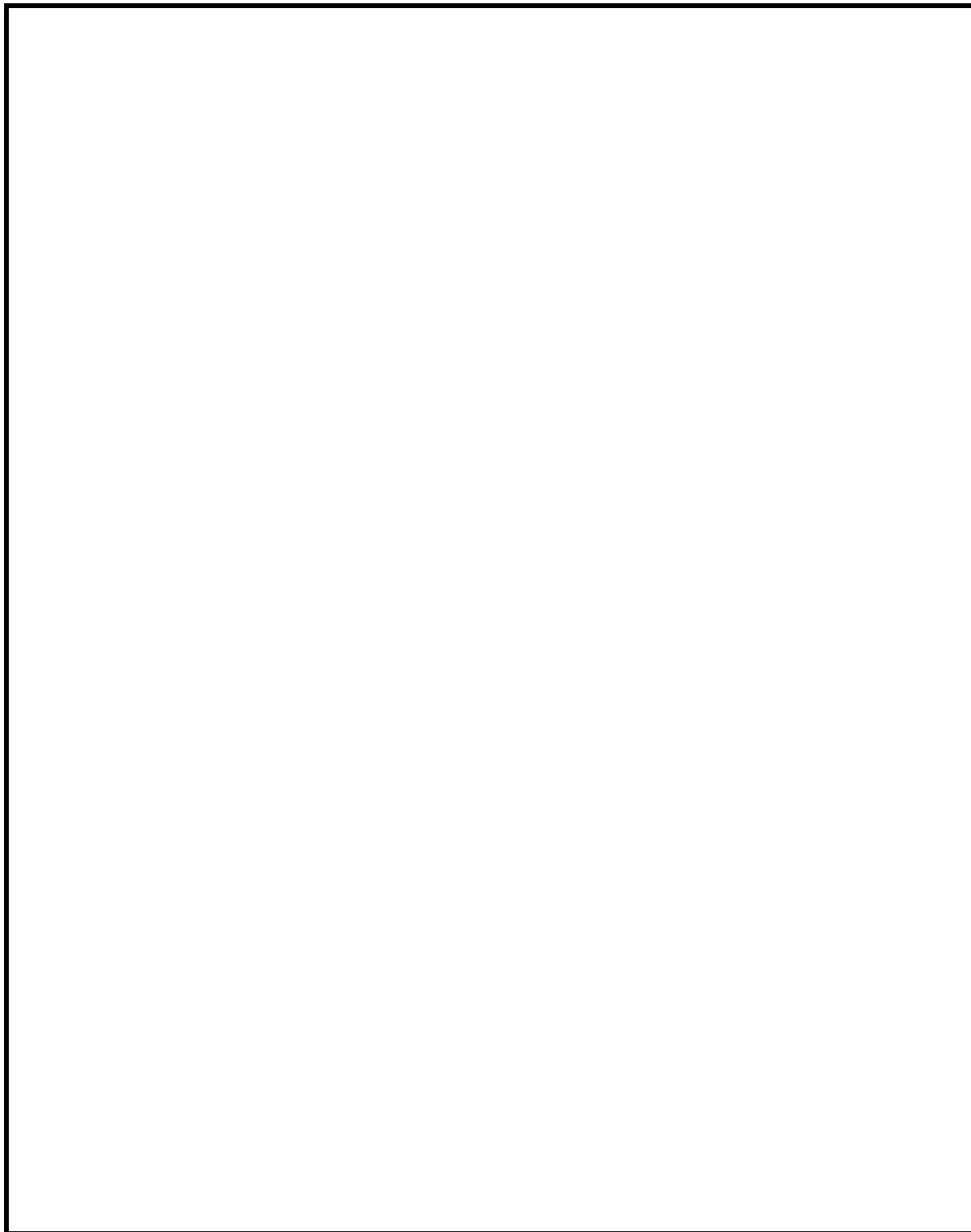

**Scheme (1)**

Table 1- The nomenclatures , physical properties of compounds (1-39)

No .	Nomenclature	Structure	Chemical formula (M.Wt.)	Yield %	Color	M.P. °C
1	Benzo[d] thiazole -2- thiol		C ₇ H ₅ NS ₂ (167.25)	85	Off White	177-179
2	S-benzo[d]thiazol-2-yl-2-chloroethanethioate		C ₉ H ₆ NO S ₂ Cl (243.73)	81	Red	98 - 100
3	S-benzo[d]thiazol-2-yl 2-(2-phenylhydrazinyl)ethanethioate		C ₁₅ H ₁₃ N ₃ O ₂ S ₂ (315.41)	80	Brown	176-178
4	S-benzo[d]thiazol-2-yl 2-(2-(hydroxy(phenyl)methyl)-2-phenylhydrazinyl)ethanethioate		C ₂₂ H ₁₉ N ₃ O ₂ S ₂ (421.54)	65	Green	130-133
5	S-benzo[d]thiazol-2-yl 2-(2-(hydroxy(4-nitrophenyl)methyl)-2-phenylhydrazinyl)ethanethioate		C ₂₂ H ₁₈ N ₄ O ₄ S ₂ (466.53)	50	Red	132-135
6	S-benzo[d]thiazol-2-yl 2-(2-(4-bromophenyl)(hydroxy)methyl)-2-phenylhydrazinyl)ethanethioate		C ₂₂ H ₁₈ N ₃ BrO ₂ S ₂ (500.43)	51	Brown	131-133
7	S-benzo[d]thiazol-2-yl 2-(2-(4-chlorophenyl)(hydroxy)methyl)-2-phenylhydrazinyl)ethanethioate		C ₂₂ H ₁₈ ClN ₃ O ₂ S ₂ (455.98)	60	brown	160-164
8	S-benzo[d]thiazol-2-yl 2-(2-(hydroxy(4-hydroxyphenyl)methyl)-2-phenylhydrazinyl)ethanethioate		C ₂₂ H ₁₉ N ₃ O ₃ S ₂ (437.53)	60	Brown	150-154
9	S-benzo[d]thiazol-2-yl 2-(2-(hydroxy(4-methoxyphenyl)methyl)-2-phenylhydrazinyl)ethanethioate		C ₂₃ H ₂₁ N ₃ O ₃ S ₂ (451.56)	66	Dark Blue	130-134
10	S-benzo[d]thiazol-2-yl 2-(2-(4-formylphenyl)(hydroxy)methyl)-2-phenylhydrazinyl)ethanethioate		C ₂₃ H ₁₉ N ₃ O ₃ S ₂ (449.55)	71	Dark Green	88-90
11	S-benzo[d]thiazol-2-yl 2-(2-(4-(dimethylamino)phenyl)(hydroxy)methyl)-2-phenylhydrazinyl)ethanethioate		C ₂₄ H ₂₄ N ₄ O ₂ S ₂ (464.60)	70	Brown	145-147

12	S-benzo[d]thiazol-2-yl 2-(2-(hydroxy(3-nitrophenyl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{22}H_{18}N_4O_4S_2$ (466.53)	68	Orange	98-100
13	S-benzo[d]thiazol-2-yl 2-(2-(hydroxy(naphthalen-2-yl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{26}H_{21}N_3O_2S_2$ (471.59)	79	brown	189-192
No.	Nomenclature	Structure	Chemical formula (M.Wt.)	Yield %	Color	M.P. °C
14	6-chlorobenzo[d]thiazole-2-thiol		$C_7H_4ClNS_2$ (201.70)	78	Gray	160-164
15	S-6-chlorobenzo[d]thiazol-2-yl 2-chloroethanethioate		$C_9H_5Cl_2NS_2O$ (278.18)	80	Off white	130-132
16	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-phenylhydrazinyl)ethanethioate		$C_{15}H_{12}ClN_3O$ S_2 (349.86)	50	Yellow	145-148
17	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(hydroxy(phenyl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{22}H_{18}ClN_3O_2S_2$ (455.98)	90	Off white	105-108
18	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(hydroxy(4-nitrophenyl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{22}H_{17}ClN_4O_4$ S_2 (500.04)	57	Yellow	108-110
19	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(4-bromophenyl)(hydroxy)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{22}H_{17}BrClN_3O_2$ S_2 (534.88)	57	Off white	124-126
20	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(4-chlorophenyl)(hydroxy)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{22}H_{17}Cl_2N_3O_2$ S_2 (490.43)	50	Yellow	240-244
21	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(hydroxy(4-hydroxyphenyl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{22}H_{18}ClN_3O_2$ S_2 (471.98)	89	Yellow	108-110
22	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(hydroxy(4-methoxyphenyl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{23}H_{20}ClN_3O_3S_2$ (486.01)	72	Yellow	180-184
23	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(4-formylphenyl)(hydroxy)methyl)-2-		$C_{23}H_{18}ClN_3O_3$ S_2 (483.99)	43	Yellow	116-118

	phenylhydrazinyl)ethanethioate					
24	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-((4-(dimethylamino)phenyl)(hydroxy)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{24}H_{23}Cl N_4O_2S_2$ (499.05)	71	dark Yellow	78-80
25	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(hydroxy(3-nitrophenyl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{22} H_{17} Cl N_4 O_4 S_2$ (500.98)	43	Yellow	110-112
26	S-6-chlorobenzo[d]thiazol-2-yl 2-(2-(hydroxy(naphthalen-2-yl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{26} H_{20} Cl N_3 O_2 S_2$ (506.04)	85	yellow	53-55
27	6-methoxybenzo[d]thiazole-2-thiol		$C_8 H_7N O S_2$ (197.28)	63	Gray	180-183
28	S-6-methoxybenzo[d]thiazol-2-yl 2-chloroethanethioate		$C_{10} H_8 NCl O_2 S_2$ (273.76)	76	yellow	160-164
No .	Nomenclature	Structure	Chemical formula (M.Wt.)	Yield %	Color	M.P. °C
29	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-phenylhydrazinyl)ethanethioate		$C_{16} H_{15} N_3 O_2 S_2$ (345.44)	50	yellow	120-124
30	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-(hydroxy(phenyl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{23}H_{21}N_3 O_3S_2$ (451.56)	77	Off white	155-157
31	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-(hydroxy(4-nitrophenyl)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{23} H_{20} N_4 O_5 S_2$ (496.56)	52	Dark yellow	175-180
32	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-((4-bromophenyl)(hydroxy)methyl)-2-phenylhydrazinyl)ethanethioate		$C_{23} H_{20} Br N_3 O_3S_2$ (530.46)	47	yellow	180-184
33	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-((4-chlorophenyl)(hydroxy)met		$C_{23}H_{20}Cl N_3O_3S_2$ (486.01)	40	white	198-200

	hyl)-2-phenylhydrazinyl)ethanethioate					
34	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-(hydroxy(4-hydroxyphenyl)methyl)-2-phenylhydrazinyl)ethanethioate	$C_{23}H_{21}N_3O_4S_2$ (467.10)	65	yellow	194-198	
35	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-(hydroxy(4-methoxyphenyl)methyl)-2-phenylhydrazinyl)ethanethioate	$C_{24}H_{23}N_3O_4S_2$ (481.59)	80	Dark yellow	168-170	
36	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-((4-formylphenyl)(hydroxymethyl)-2-phenylhydrazinyl)ethanethioate	$C_{24}H_{21}N_3O_4S_2$ (479.57)	60	yellow	180-182	
37	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-((4-formylphenyl)(hydroxymethyl)-2-phenylhydrazinyl)ethanethioate	$C_{25}H_{26}N_4O_3S_2$ (494.63)	66	yellow	120-122	
38	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-(hydroxy(3-nitrophenyl)methyl)-2-phenylhydrazinyl)ethanethioate	$C_{23}H_{20}N_4O_5S_2$ (496.56)	45	Off white	227-230	
39	S-6-methoxybenzo[d]thiazol-2-yl 2-(2-(hydroxy(naphthalen-2-yl)methyl)-2-phenylhydrazinyl)ethanethioate	$C_{27}H_{23}N_3O_3S_2$ (501.62)	60	yellow	148-150	

Result and Discussion

2-MBT and some of its derivatives was obtained from the reaction of aniline or its derivatives with carbon disulfide in absolute ethanol and in presence of sulphure by using closed system . This method was selected because it gave 2-MBT and its derivatives in a good yield and high purity.[28]

According to the equation below:



* R = -H , -Cl , -OCH₃

The structure of the compound was confirmed from its melting point table (1) and FTIR spectrum table (2) in addition to the C.H.N.S analysis table (3). The FTIR spectrum of the compounds (1,14,27) show a stretching band at (3097-3020) cm^{-1} (C-H) aromatic; (1590) cm^{-1} ; (C=N) thiazole;(736-696) cm^{-1} (C-S), and disappearance of the two absorption band in the range of (3387, 3286), (3363,3194) cm^{-1} which could be attributed to asymmetric and symmetric stretching vibration (NH_2) group of aniline. Fig (2) show The FTIR spectrum for compound (1) These bands and others are shown in table (2) . Then reaction 2-mercaptobenzothiazole and some its derivatives with chloroacetyl chlorid in alkali media was used to prepare the compounds (2,15,28). The halogroup in chloroacetylchlorid is good leaving group and sulfur compounds are a good nucleophile Thus, the reaction is a typical of the nucleophilic substitution reaction of the thiol group , where the halo group could be replaced easily in this reaction to get good yield according to the mechanism below [29].

* R = -H , -Cl , -OCH₃

The FTIR spectrum showed a strong stretching band at (3090-3020) cm^{-1} (C-H) aromatic ; 1730-1724 cm^{-1} for U(C=O) ; (695 -601) cm^{-1} U(C-S) ; (1626 -1616) cm^{-1} for U(C=N) thiazole [30] . Figure (3)and(4) show the FTIR spectrum for compouds (2)and (15) respectively. The prepare Hetrocyclic compound (triazine) ; the phenyl hydrazide was seen suitable chiron for this synthetic approach . 1- chloro acetyle -2- MBT and its derivatives was stirred with phenyl hydrazine to gave the expected phenyl hydrazide (3,16,29) as shown below :

D
* R = -H , -Cl , -OCH₃

The purity and structure of (3,16,29) were confirmed by FT IR spectroscopy. FT IR showed band at 3210 cm^{-1} due to(N-H). The spectrum also showed a characteristics aromatic band at 3057 cm^{-1} U (C-H) The IR spectra also showed strong band of at 1722- 1700 cm^{-1} U (C=O) and 1600 cm^{-1} characteristics of the 2-MBT Nuclues. Figure (5) show the FTIR spectrum for compouds (3). Besides the multiple pharmacological activities of compounds possessing the 2-MBT nucleus, hydrazone compounds may be displayed tuberculostatics and anti convulsant activity, this observation prompted synthesis of some hydrazones compounds. The new derivatives (4-13) , (17-26) , (30-39) were obtained good yield through the reaction of phenyl hydrazio acetyl-2-MBT and some of its derivatives (3,16,29) with different aromatic aldehydes scheme (1), Synthesis of compound (4-13) , (17-26) , (30-39) involved nucleophilic attack [31] of amino group in compound (3,16,29) on carbonyl group in different aromatic aldehyde according to mechanism below:



* R = -H , -Cl , -OCH₃

Ar = different aromatic aldehydes.

FTIR spectrum showed strong stretching band at (3500-3300 cm^{-1}) broad U(O-H) ; 3325 cm^{-1} U (N-H); 3025 cm^{-1} U(C-H) aromatic and 1733-1700 cm^{-1} for U(C=O) . These bands and others are shown in table-2&3.

Table 2- FT-IR spectral data of compounds (1-39).

Comp. NO.	Chemical structure	U N-H cm^{-1}	U C=O cm^{-1}	U O-H cm^{-1} (broad)	U C=N Thiazole cm^{-1}	Other Bands cm^{-1}
1		—	—	—	1589	UC-S 736-696 U 1522,1445
2		—	1730	—	1580	UC-Cl 594
3		3213	1716	—	1589	UC-N 1313-1271
4		3325	1712	3500-3300	1546	—
5		3303	1700	3585-3400	1596	σ NO ₂ 1518asym 1341sym p-position for NO ₂ 812
6		3200	1720	3500-3300	1546	UC-Br 660 p-position for Br 812
7		3211	1730	3514-3375	1589	UC-Cl 595 p-position for Cl 812
8		3230	1730	3380-3430	1580	p-position for OH 812
9		3340	1730	3500-3400	1600	σ C-O-C 1250
10		3299	1733	3494-3417	1577	—
11		3313	1730	3477-3396	1596	U C-N 1292-1259
12		3289	1725	3400-3300	1611	two band (m-position) 750, 720
Comp. NO.	Chemical structure	U N-H cm^{-1}	U C=O cm^{-1}	U O-H cm^{-1} (broad)	U C=N Thiazole cm^{-1}	Other Bands cm^{-1}
13		3272	1739	3564-3365	1596	—
14		—	—	—	1612	UC-Cl 626

15		—	1724	—	1600	UC-Cl 574
16		3303	1700	—	1600	UC-Cl 572
17		3225	1710	3500 3300	1633	—
18		3200	1720	3500 3300	1614	σ NO ₂ 1520 1300
19		3290	1700	3400 3300	1600	—
20		3200	1701	3500 3300	1612	—
21		3300	1700	3450 3350	1575	σ OH 3380
22		3250	1710	3500 3300	1580	—
23		3200	1724	3500 3300	1670	σ 1701
24		3240	1730	3500- 3300	1600	—
25		3236	1722	3400- 3330	1633	two band (m-position) 750, 720
26		3325	1726	3550- 3460	1633	UC-Cl 601
Comp. NO.	Chemical structure	U N-H cm⁻¹	U C=O cm⁻¹	U O-H cm⁻¹ (broad)	U C=N Thiazole cm⁻¹	Other Bands cm⁻¹
27		—	—	—	1546	σ C-O-C 1244
28		—	1726	—	1612	σ C-O-C 1255 UC-Cl 613
29		3429	1722	—	1614	σ C-O-C 1249
30		3240	1700	3500- 3300	1602	—
31		3230	1720	3434- 3300	1600	σ NO ₂ 1521 1346
32		3210	1730	3500- 3389	1590	UC-Br 615 σ C-O-C 1247

33		3236	1730	3400-3330	1616	UC-Cl 619
34		3250	1720	3545-3390	1595	σ C-O-C 1247
35		3250	1712	3400-3330	1602	σ C-O-C 1251
36		3210	1718	3370-3502	1580	σ C-O-C 1247
37		3200	1720	3500-3300	1590	UC-N 1299 σ C-O-C 1247
38		3250	1730	3400-3350	1614	two band (m-position) 750, 720
39		3300	1720	3525-3400	1612	—

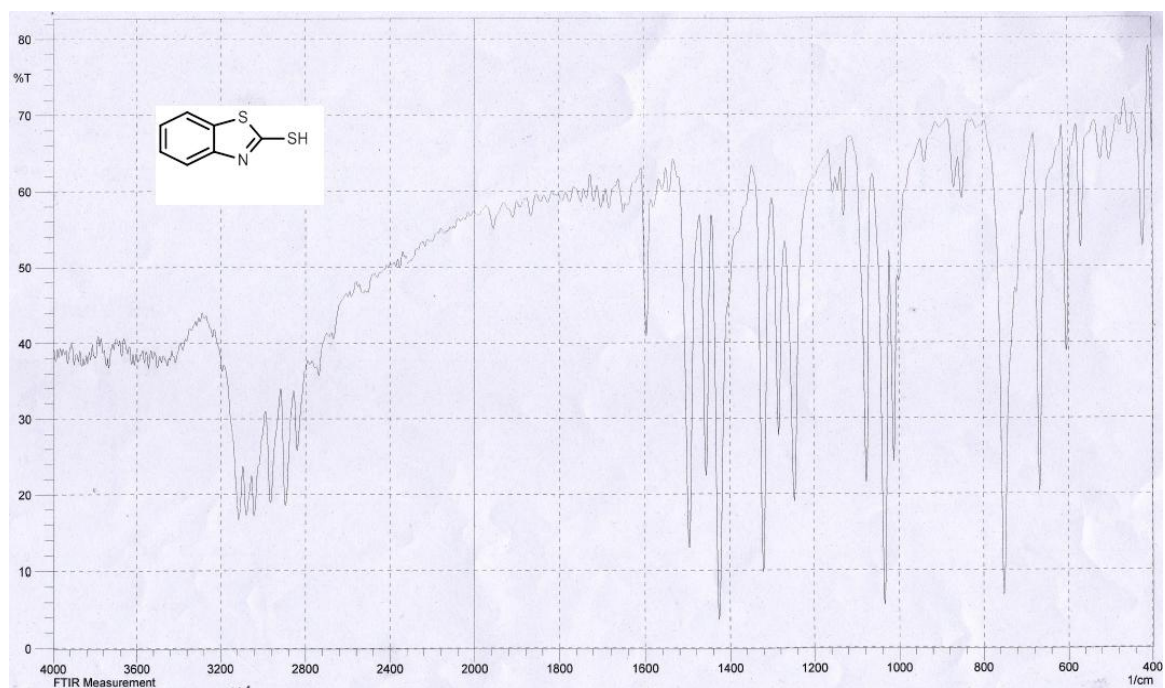


Figure 2- FTIR spectrum for compound (1).

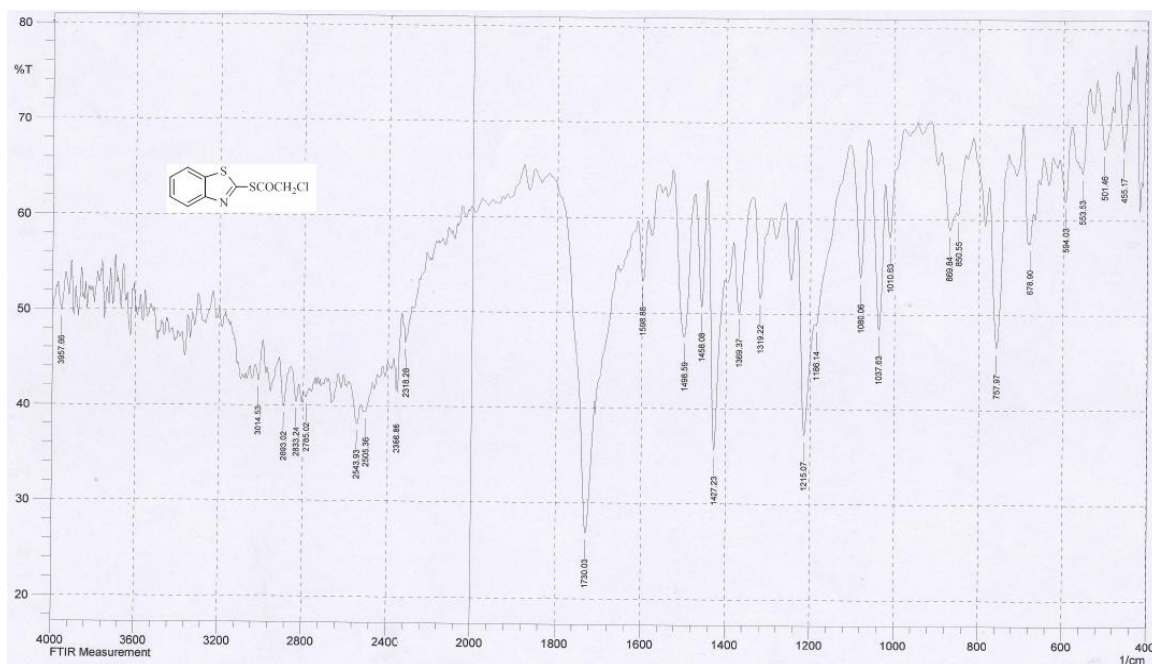


Figure 3- FTIR spectrum for compound (2)

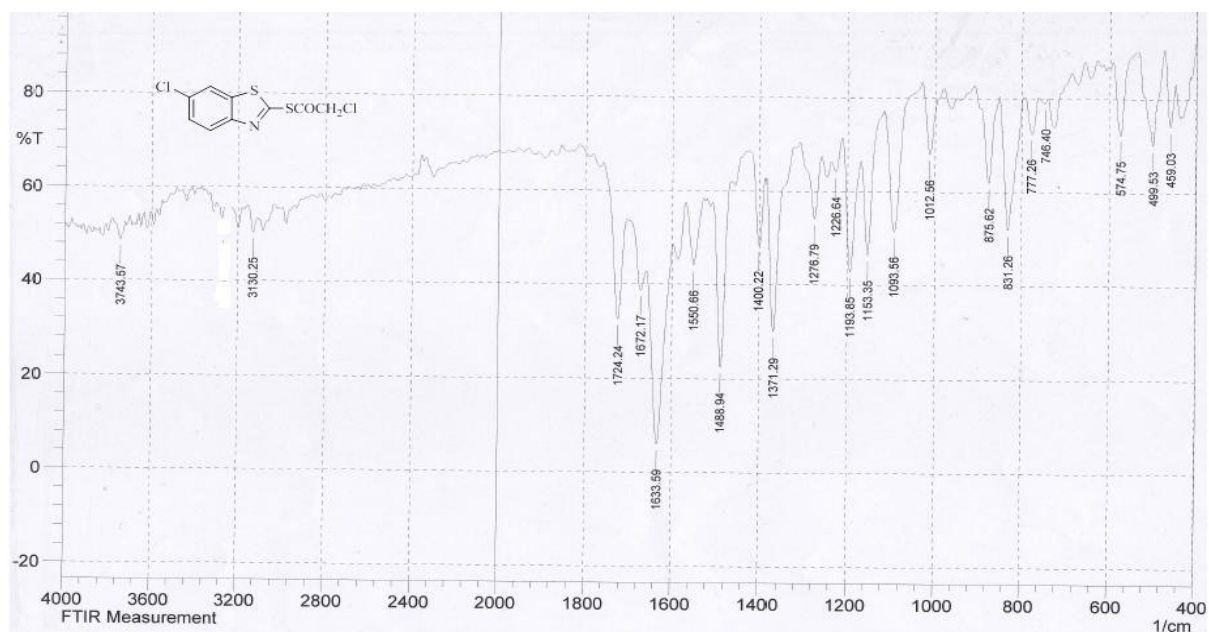


Figure 4- FTIR spectrum for compound (15).

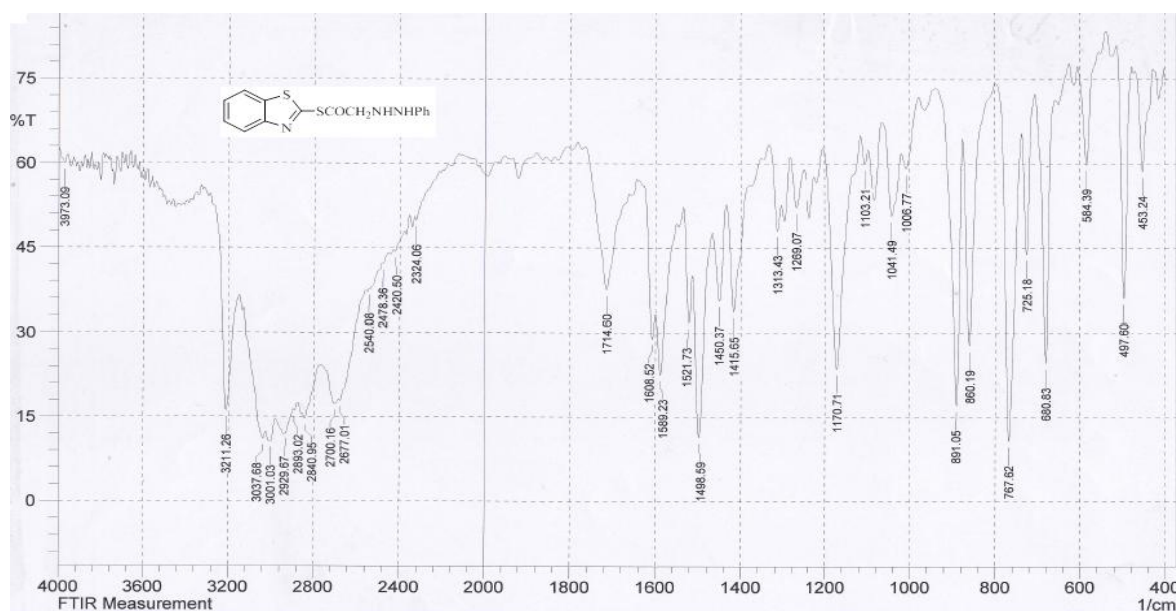


Figure 5- FTIR spectrum for compound(3)

Table 3- The C.H.N.S analysis of some prepared compounds

Comp. NO.	Molecular Formula	Calculate %				Found %			
		C	H	N	S	C	H	N	S
1	C ₇ H ₅ NS ₂	50.27	3.01	8.37	38.34	50.33	2.90	8.11	38.01
2	C ₉ H ₆ NOS ₂ Cl	44.35	2.48	5.75	26.31	44.01	2.11	5.56	26.11
3	C ₁₅ H ₁₃ N ₃ OS ₂	57.12	4.15	13.32	20.33	56.99	3.95	13.20	20.21
5	C ₂₂ H ₁₈ N ₄ O ₄ S ₂	56.64	3.89	12.01	13.75	56.49	3.79	11.91	13.66
8	C ₂₂ H ₁₉ S ₂ N ₃ O ₃	60.39	4.38	9.60	14.66	60.12	4.20	9.50	14.59
9	C ₂₃ H ₂₁ N ₃ O ₃ S ₂	61.18	4.69	9.31	14.20	60.99	4.58	9.22	14.01
10	C ₂₃ H ₁₉ N ₃ O ₃ S ₂	61.45	4.26	9.35	14.27	61.29	4.01	9.29	14.26
11	C ₂₄ H ₂₄ N ₄ O ₂ S ₂	62.04	5.21	12.06	13.80	61.99	5.19	12.03	13.77
12	C ₂₂ H ₁₈ N ₄ O ₄ S ₂	56.64	3.89	12.01	13.75	56.59	3.81	11.99	13.69
13	C ₂₆ H ₂₁ N ₃ O ₂ S ₂	66.22	4.49	8.91	13.60	66.19	4.39	8.87	13.55
27	C ₈ H ₇ NOS ₂	48.71	3.58	7.10	32.51	48.60	3.53	7.04	32.48
29	C ₁₆ H ₁₅ N ₃ O ₂ S ₂	55.63	4.38	12.16	18.56	55.59	4.35	12.16	18.55
30	C ₂₃ H ₂₁ N ₃ O ₃ S ₂	61.18	4.67	9.31	14.20	61.16	4.66	9.30	14.18
31	C ₂₃ H ₂₀ N ₄ O ₅ S ₂	55.63	4.06	11.28	12.91	55.62	4.04	11.25	12.89
34	C ₂₃ H ₂₁ N ₃ O ₄ S ₂	59.08	4.53	8.99	13.72	59.07	4.50	8.97	13.72
36	C ₂₄ H ₂₁ N ₃ O ₄ S ₂	60.11	4.41	8.76	13.37	60.09	4.39	8.72	13.35
37	C ₂₅ H ₂₆ N ₄ O ₃ S ₂	60.71	5.30	11.33	12.97	60.66	5.28	11.33	12.96
38	C ₂₃ H ₂₀ N ₄ O ₅ S ₂	55.63	4.06	11.28	12.91	55.61	4.04	11.27	12.89

References:

1. El-Sayed R., 2006. Synthesis, antibacterial and surface activity of 1,2,4-triazole derivatives. *Grasas Y Aceites*, 57(2), pp:180-188.
2. Vedavathi M., B. Somashekar, G. M. Sreenivasa, E. Jayachandran. 2010. Synthesis, Characterization and Anti-microbial activity of fluoro benzothiazole incorporated with 1,3,4-Thiadiazole. *J. Pharm. Sci. & Res.*, 2(1), pp: 53-63.
3. Gurupadaya BM, Gopal M, Padmashali B, Vaidya VP. 2005. Synthesis and biological activities of fluoro benzothiazoles. *Int J Heterocyclic Chem*, 15, pp: 169-172.
4. Geoffrey W, Tracey DB, Patrizia D, Angela S, Dong-Fang S, Andrew D, Westwell MF, Stevens G, 2000. Antitumour Benzothiazoles. Part 10: The Synthesis and Antitumour Activity of Benzothiazole Substituted Quinol Derivatives. *Bioorg. & Med. Chem. Lett.* 10, pp: 513-515.

5. Kochichiro Y, Katsumi G, Kazuya Y, Tominori M and Goro T. **2007**. Synthesis and evaluation of novel benzothiazole derivatives against human cervical cancer cell lines, *Int. J. Pharm. Sci.*; 69 (1) , pp: 46-50.
6. Bhusari KP, Khadekar PB, Umathe SN, Bahekar RH and Rao AR, **2000**. synthesis and anti-tubercular activity of some substituted 2-(4- aminophenyl sulphonamide) Benzothiazoles. *Indian J. Hetrocyclic Chem.* , 9, pp: 213-216.
7. Klein LL, Yeuns CM, Weissing DE, Lartey PA, Tonaka SK, Plattner JJ and Mulford DJ, **1994**. Synthesis and antifungal activity of 1,3,2-benzodithiazole S-oxides. *J Med Chem*,37, pp: 572-578.
8. Rajeeva B, Srinivasulu N, Shantakumar S. **2009**. Synthesis and Antimicrobial activity of some new 2-substituted benzothiazole derivatives. *E-Journal of Chemistry*; 6(3), pp:775-779.
9. Stanton HLK, R Gambari, Chung HC, Johny COT, Filly C, Albert SCC., **2008**. Synthesis and anti-cancer activity of benzothiazole containing phthalimide on human carcinoma cell lines. *Bioorg Med Chem.*,16,PP:3626-3631.
10. Pattan S, Suresh C, Pujar V, Reddy V, Rasal V, Koti B., **2005**. Synthesis and antidiabetic activity of 2-amino[5''(4-sulphonylbenzylidene)-2, 4-thiazolidinenone]-7-chloro-6-flurobenzothiazole. *Ind J Chem.*, 44B, pp:2404-2408.
11. Kaur H., S. Kumar, I. Singh, K. K. Saxena, A. Kumar. **2010**. Synthesis, Characterization and Biological activity of various substituted benzothiazole derivatives. *Digest J. Nanomaterials and Biostructures* ,5(1), pp: 67-76.
12. Mohammed Afzal Azam and Bhojraj Suresh. **2012**. Biological Activities of 2-Mercaptobenzothiazole Derivatives: A Review. *Sci Pharm.*, 80(4), PP: 789–823.
13. Holbova E, Sidoova E, Zemanova M, Drobnicova I. **1990**. Synthesis 3-(2-Alkylthio-6-benzothiazolylamino-methyl)-6-bromo-2-benzothiazohnones and their antimicrobial activity. *Chem Papers.*,44, pp:363–368.
14. GALSTON, A. W., BAKER, R. S., and KING, J. W. **1953**. Benzimidazole and the geometry of cell growth. *Physiol. Plantarum* ,6, pp: 863-872.
15. Metzger, J. V., **1984**, In Comprehensive Heterocyclic Chem. Chapter on Thiazole and Benzothiazole Derivatives Katritzky, A.; Rees, C. W., Eds. Pergamon,6, pp:330-331
16. Refaey, S.; Taha, F.; Abd El-Malak, A., **2006**., Corrosion and Inhibition of 316L Stainless Steel in Neutral Medium by 2-Mercaptobenzothiazole. *Int. J. Electrochem. Sci.*, 1, pp:80-91.
17. Wang, L., **2001**. Evaluation of 2-Mercaptobenzothiazole as Corrosion Inhibitor for Mild Steel in Phosphoric Acid, *Corros. Sci.*, 43, pp:2281.
18. Wang, L.; Pu, J.; Luo, H., **2003**. Corrosion Inhibition of Zing in Phosphoric Acid Solution by 2-Mercaptobenzothiazole"; *Corros. Sci.*, 45, pp:77.
19. Norford, D.; Meaten, D.; Cullen, J.; Collins, J., **1993**. Pituitary and Thyroid Gland Lesions Induced by 2-Mercaptobenzothiazole Inhalation in Male Fischer-344 Rats. *Soci, Toxicol-Patho.*,21(5), pp:456-460.
20. Salman, M.; Abu-Krishna, M.; El-Sheshtawy, H., **2004**. Charge Transfer Complexes of MBI with α - and Π -Electron Acceptor"; *Cand. J. Analy. Sci. Spect.*, 49(5), pp:282-289.
21. Saxena, D.; Kajuria, R.; Suri, O., **1982**. Synthesis and Spectral Studies of 2-Mercaptobenzothiazole Derivatives"; *J. Hetro. Chem.*, 19, pp:681-689.
22. Berchmans, S.; Arivukkodi, S.; Yegnaraman, N., **2000**. Self Assembled Monolayer of 2-Mercaptobenzothiazole on Gold Stripping Volumetric Determination of Hg(II). *Electro. Commun.*, 2, pp:226-230.
23. Chalapathi, K.; Rameshbabu, L.; Madhu, P.; Maddaiah, G., **2010**. 2-Mercapto benzothiazole Immobilized with Amberlite Xad-2 Using as Solid Phase Extractor for the Determination of Fe(II), Cu(II), & Cd(II)". *Adv. Appl. Sci, Res.*, 1(2), pp:27-35.
24. Lee JH, Kim JD. **1997**. S-Acyl derivatives of benzothiazole-2-thiol: A convenient method for the synthesis of amides and carbamates. *Bull Korean Chem Soc.*,18, pp:442–443.
25. Ahlam Jameel Hamood, **2006**. Synthesis of 2-Mercaptobenzothiazole and Some of its derivatives and study it effect on some strains of Bacteria. M.Sc. Thesis. Department of Chemistry ,College of Science ,University of Baghdad, Baghdad, Iraq, pp:24.
26. Yadav R., Srivastava S D & Srivastava S K. **2005**. Synthesis, antimicrobial and anti-inflammatory activities of 4-oxothiazolidines and their 5-arylidenes. *Indian Journal of Chemistry* ,44B : pp:1262-1266 .

27. Ahamed L. S. **2005**. Synthesis And Biological Activity study of new C-and N-substituted Phenothiazine Derivatives .M.Sc. Thesis, Department of Chemistry, College of Science, University of Baghdad .Baghdad, Iraq, pp:20.
28. Hamood A. J. **2006**. Synthesis of 2-Mercaptobenzothiazole and Some of its derivatives and study it effect on some strains of Bacteria. M.Sc. Thesis, Department of Chemistry ,College of Science ,University of Baghdad, Baghdad, Iraq, pp:39.
29. Suaad, M.H. Al-Majidi and Khitam, T.A., Al- Sultani. **2010**. Synthesis and antimicrobial activity of some new acetylenic amine of istin derivatives. *J. Al-Mustansiryia Sci.* 21 (4), pp: 61-72.
30. Sliverstien, R.M., and Websters X., **1998**, *Spectrometric Identification of organic compounds*, 6 th Ed., John Wiely and Sons, New York.
31. Vogel A., **1989**. *Vogel 's A Textbook of Practical Organic Chemistry*, 5th (Ed.), revised by B. Furniss, A. Hannaford, P. Smith, and A. Tatchell, Longman group limited, London, UK,.