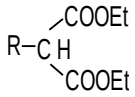
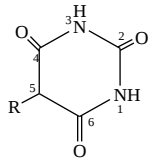
:Table 2.4.a: Infrared spectral data of intermediate substituted diethyl malonate derivatives



Cpd. No	R	C=O .st.vib	C=C–H St.vib	C–H	C=C St.vib	.C-O st.vib	.O-H st.vib
Ia	$-C_2H_5$	v),sharp 1738) and sh. 1740	-	St.vib 2985 and sh. 2980 ben. 1465,1372	-	1189	m), sharp,3466)
Ib	$-C_6H_5-CH_2$	v),sharp 1733)	3063	St.vib 2998 and sh. 2938 ben. 1450,1370	1600-1450	1229	s), sharp,3470)
II	$-C_6H_5$	v),sharp 1735)	sh. 3050	St.vib 2983 and sh.2980 ben. 1455,1369	1600-1455	1219	s), sharp,3465)
III	$-EtOOC)_2CH)$	v),broad 1736)	-	St.vib 2908 and sh.2877 ben. 1469,1369	-	1190,1147	m), sharp3450)
VI a	$-CH_3-CO$	v),sharp1738and) 1626	-	St.vib 2980 ben. 1371	-	1180	m), sharp3633)
VI b	$-C_6H_5-CO$	v),broad 1691)	3050	St.vib 2986 ben. 1452,1324	1601-1452	1070	m), broad,) 3409

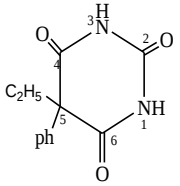
St.vib= stretching vibration, sh. = shoulder; ben. = bending vibration v, s, m, w = very strong, strong, medium, and weak absorption respectively

: Table 2.4.b: Infrared spectral data of 5-substituted pyrimidine-2,4,6-trione derivatives



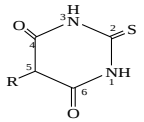
Cpd. No	R	N-H	C=O .st.vib	C–H	C=C St.vib	C–H st.vib	O-H .st.vib	C-O .st.vib
Va	$-C_2H_5$	st.vib. 3150 ben. 1520	v), three bands) 1729, 1700,1710	st.vib. 2983 ben. 1460,1375	-	-	broad,(m), 3465	sharp, 1296
Vb	$-C_6H_5-CH_2$	st.vib. 3100 ben. 1520	v), two bands) 1720,1705	st.vib. 2851 ben. 1442,1367	1497-1409	3075	-	sharp,1294
Vc	$-C_6H_5$	st.vib. 3150 ben. 1598	v), two bands) 1700,1626	st.vib. 2985 ben. 1456,1406	1598-1456	3030	w),sharp) 3450	sharp,1282
Vd	$-CH_3-CO$	st.vib. 3100 ben. overlap	v), broad 1700)	st.vib. 2990 ben. 1456,1400	-	-	m),sharp) 3358	sharp,1161
Ve	$-C_6H_5-CO$	st.vib. 3150 ben. 1598	v), two bands) 1704,1629	st.vib. 2900 ben. 1471,1349	1598-1544	3050	-	sharp,1285
Vf	H	st.vib.3563 and 3098 ben. 1619	s) broad 1713)	st.vib. 2876 and sh 2800 ben. 1350	-	-	sharp, 3477	sharp,1248

: (Table 2.4.c: Infrared spectral data of 5-ethyl -5-phenyl pyrimidine-2,4,6-trione (phenobarbitone, standard sample



Cpd. No	R	N-H	.C=O st.vib	C –H	C=C	=C–H st.vib	O-H st.vib	C-O st.vib
STD	-C_6H_5- , C_2H_5	st.vib. 3183 ben. 1575	v), two bands) 1696 and 1667	st.vib. 2970 ben. 1374	1462-1413	3059	-	-

-:Table 2.4.d: Infrared spectral data of the 5-substituted pyrimidine-2-thio- 4,6- dione



Cpd. No	R	N-H	.C=O st.vib	C=S st.vib	C –H	C=C St.vib	C–H st.vib	O-H .st.vib	.C-O st.vib
VI a	$-C_2H_5$	w),st.vib.) 3100 ben. 1564	v), three bands) 1700, 1650 and 1632	1243	st.vib. 2896 ben. 1442,1401	-	-	w), broad) 3480	v),sharp) 1241
VI b	$-C_6H_5-CH_2$	w),st.vib.) 3100 ben. 1616	v), two bands) 1730 and 1737	1215	st.vib. 2986 ben. 1453	1616-1453	3050	-	sharp1303
VI c	$-C_6H_5$	st.vib. 3100 ben. Overlap	v), two bands) 1620 and 1564	1251	st.vib. 2796 ben. 1441,1376	1441-1376	3050	-	v),sharp) 1289
VId	$-EtOOC)_2CH$)	st.vib. 3051 ben. 1570	v), three bands) 1735,1682,1570	1181	st.vib. 2901 ben. 1435,1368	-	-	-	m),sharp) 1278
VI e	$-C_3H_2N_2SO_2-CH$	st.vib. 3174 .ben.1580	v), two bands) 1734 and 1615	1175	st.vib. 2990 ben. 1470,1415	-	-	sharp,(v), 3385	v),sharp) 1290
VI f	$-CH_3-CO$	st.vib. 3220 ben. 1592	V), three bands) 1722,1710,1620	1162	st.vib. 2804 ben. 1468,1407	-	-	sharp,(s), 3654	v),sharp) 1167
VI g	$-C_6H_5-CO$	st.vib. 3398 ben. 1598	v), two bands) 1724 and1661	1173	st.vib. 2928 ben. 1447	1598-1447	3050	broad,(s), 3398	s),sharp) 1183
VIh	H	st.vib. 3423,3108	v), two bands) 1702 and 1626	sharp peak 1187	v), sharp,) st.vib. 2887	-	-	sharp,(m), 3423	s), sharp) 1279

		ben. 1532			ben. 1371				

:Investigation of keto-enol phenomena using infrared spectra

Table 2.4.e.i: infrared spectral study of keto-enol tautomersim in diethyl phenyl malonate (II) (as a liquid film using CCl_4 :(and ethanol as solvents

C_6H_5-CH$(CO_2Et)_2$

Group / vibration	liquid film using CCl_4 cm^{-1}	liquid film using Et OH cm^{-1}
C—H	st.vib. 3050	st.vib. 3050
C—H	st.vib. 2969	st.vib. 2983
C=O	st.vib. 1737(sh), and 1750 sharp	(st.vib. 1735 (b
C=C	st.vib. three peaks, 1600-1460	st.vib. three peaks, 1600-1460
C—H	ben. 1452	ben. 1452
O-H	-	st.vib.3465

:(Table 2.4.e.ii: infrared spectral study of keto-enol tautomersim in pyrimidine-2,4,6- trione (Vf) (using KBr disk

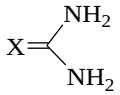
.Concentration / Group st.vib	1000µg/100mg	100µg/100mg	10µg/100mg	1.0µg/100mg
.O-H st.vib	s)sharp 3477)	m),sharp 3478)	m),sharp 3477)	-
.C=O st.vib	s)broad 1713)	s), 1704 and two (sh)) 1700 and 1740	s) 1714 and three (sh):) .1700, 1730 and 1740	three peaks, 1700, 1716and 1740, (sh):1750

:Table 2.4.f.i: infrared spectral of diethyl malonate

$CH_2(COOEt)_2$

Group / vibration	cm^{-1}
C–H	st.vib. 2985 and sh; bending, 1467,1372
C=O	st.vib. 1736
C-O	st.vib. 1151
O-H	st.vib. 3464

:Table 2.4.f.ii: infrared spectral of urea and thio-urea



X = S , O

Group / vibration	cm^{-1}
N-H	St.vib. two bands, 3445 and 3347; ben. 1600 St.vib. three bands, 3383, 3276 and 3177; ben. 1616
C=O	st.vib. 1682
C=S	st.vib. 1084