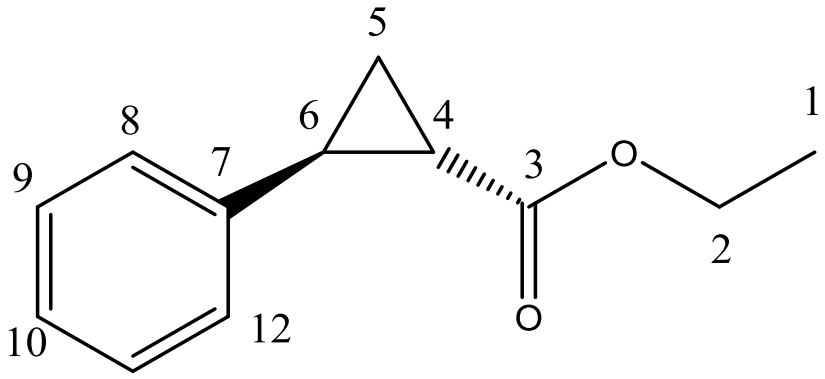
X7 (backwards)

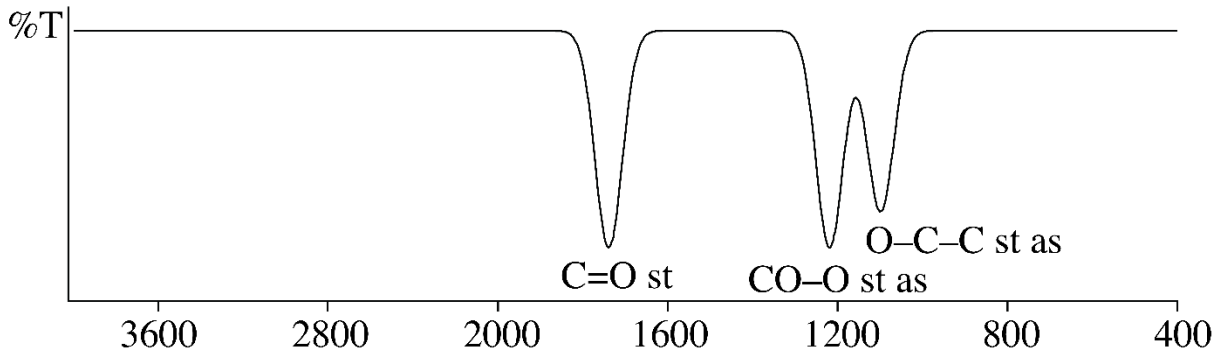


Chemical Formula: $C_{12}H_{14}O_2$
Molecular Weight: 190.24

IR

≈ 3000 cm^{-1}	C-H st. (sp^2, sp^3)
2000-1800 cm^{-1}	Overtone and combination band of bending vibration of aromatic C-H "benzene finger")
1720 cm^{-1}	C=O st. (Ester)

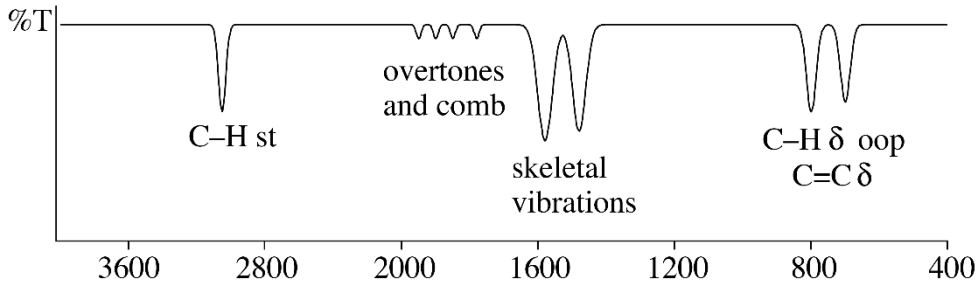
7.11.4 Esters and Lactones



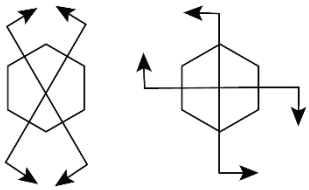
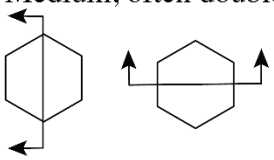
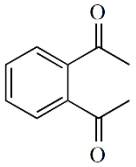
1600, 1500 cm^{-1} Skeletal vibrations aromatic ring

MS

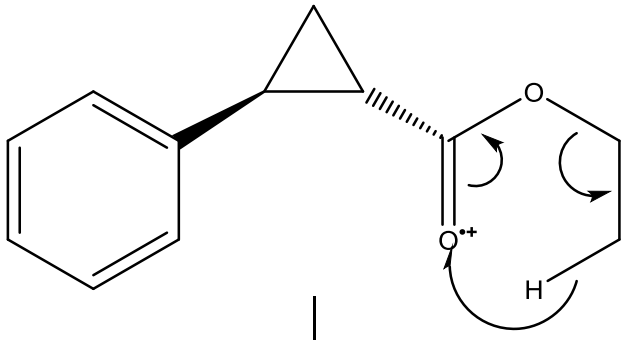
7.5 Aromatic Hydrocarbons



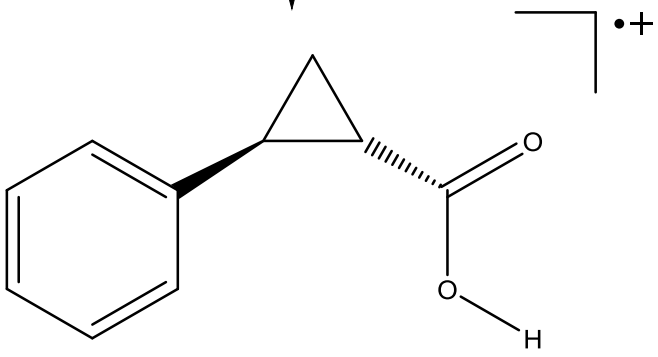
Typical Ranges ($\tilde{\nu}$ in cm^{-1})

Assignment	Range	Comments
ar C–H st	3080–3030	Often numerous bands; in the same range also CH st of alkenes and small rings
ar C–C	1625–1575	 Medium, often doublet; generally weak in benzene derivatives having a center of symmetry in the ring
		In the same range: C=C st, C=N st, C=O st, N=O st, C–C in heterocyclics, NH δ
	1525–1450	Medium, often doublet:  Weak in: 
		In the same range: C=O st, N=O st, C–C in heterocyclics, B–N st, CH_3 δ, CH_2 δ, NH δ
comb	2000–1650	Very weak; useful for determining substitution patterns in 6-membered aromatic rings
		In the same range: C=O st, B–H···B st, N^+–H st, H_2O δ
ar C–H δ ip	1250–950	Numerous bands of variable intensity; of no practical significance. May be very strong in Raman and, thereby, indicative of substitution type

m/z 162



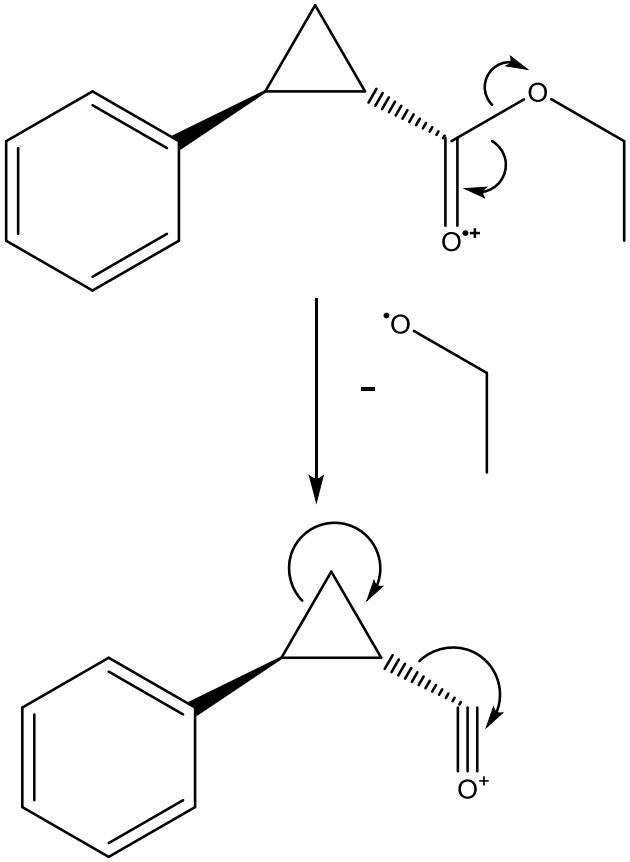
McLafferty rearrangement



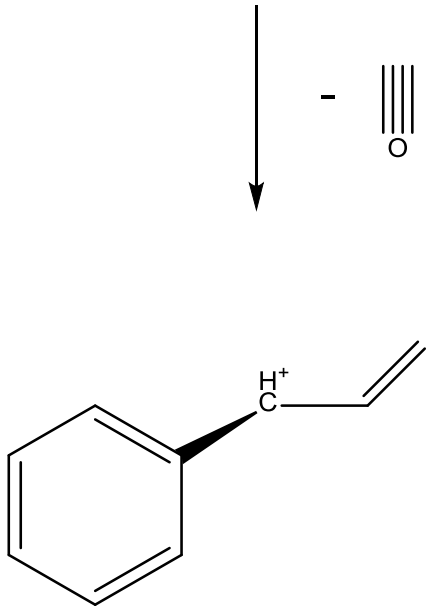
Molecular Weight: 162.19

Molecular Weight: 28.05

m/z 145 & 117

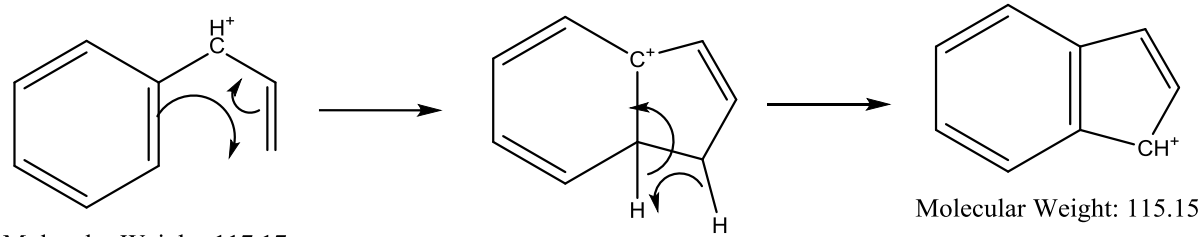


Molecular Weight: 145.18



Molecular Weight: 117.17

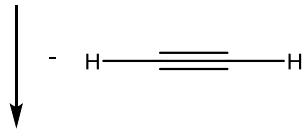
m/z 115 & 91

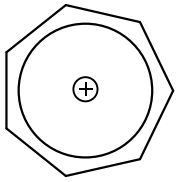


Molecular Weight: 117.17

Molecular Weight: 117.17

Molecular Weight: 115.15

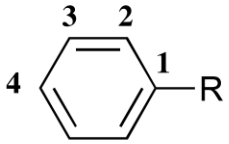




Molecular Weight: 91

^{13}C-NMR

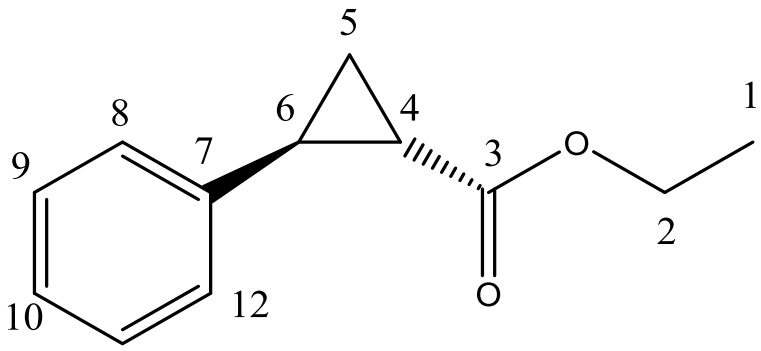
Effect of Substituents on ^{13}C Chemical Shifts of Monosubstituted Benzenes (δ in ppm)



$$\delta_{C_i} = 128.5 + Z_i$$

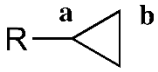
	Substituent R	Z_1	Z_2	Z_3	Z_4
C	$-CH_3$	9.2	0.7	-0.1	-3.0
	$-CH_2CH_3$	11.7	-0.6	-0.1	-2.8
	$-CH_2CH_2CH_3$	10.3	-0.2	0.1	-2.7
	$-CH(CH_3)_2$	20.2	-2.2	-0.3	-2.8
	$-CH_2CH_2CH_2CH_3$	10.9	-0.2	-0.2	-2.8
	$-C(CH_3)_3$	18.6	-3.3	-0.4	-3.1
	–cyclopropyl	15.1	-3.3	-0.6	-3.6
	–cyclopentyl	17.8	-1.5	-0.4	-2.9
	–cyclohexyl	16.3	-1.8	-0.3	-2.8

$\delta_7 = 128.5 + 15.1 = 143.6$
$\delta_{8/12} = 128.5 - 3.3 = 125.2$
$\delta_{9/11} = 128.5 - 0.6 = 127.9$
$\delta_{10} = 128.5 - 3.6 = 124.9$



Chemical Formula: $C_{12}H_{14}O_2$
Molecular Weight: 190.24

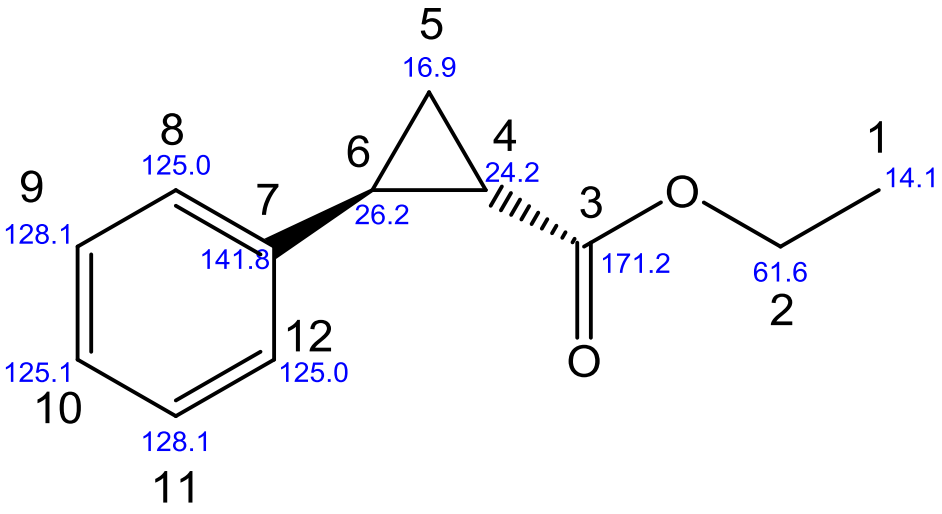
^{13}C Chemical Shifts of Monosubstituted Cyclopropanes (δ in ppm)



	Substituent R	a	b	other
	–H	-2.8	-2.8	
C	$-CH_3$	4.9	5.6	CH_3 19.4
	$-CH_2CH_3$	12.8	4.1	CH_2 27.8, CH_3 13.6
	$-CH_2CH_2CH_2CH_3$	10.9	4.4	1-CH_2 34.7, 2-CH_2 32.0
	$-C(CH_3)_3$	22.7	0.3	C 29.3, CH_3 28.2
	$-CH_2Cl$	13.6	5.5	CH_2 50.3
	$-CH_2OH$	12.7	2.2	CH_2 66.5
	$-CH{=}CH_2$	14.7	6.6	CH 142.4, CH_2 111.5
	–phenyl	15.3	9.2	C 143.9, CH 125.3–128.2
X	–Cl	27.3	8.9	
	–Br	14.2	9.1	
	–I	-20.1	10.4	
O	–OH	45.7	6.8	
N	$-NH_2$	24.0	7.4	
	$-NO_2$	54.3	11.7	
	$-C{\equiv}N$	-4.5	6.2	CN 121.5
O	–CHO	22.7	7.4	CO 202.1
‖	$-COCH_3$	20.1	9.6	CO 207.3, CH_3 29.1
C	–CO–phenyl	17.1	11.5	
	–COOH	12.7	8.9	CO 181.6
	$-COOCH_3$	12.2	7.7	CO 174.7, CH_3 51.1

δ (ppm)	DEPT	Assignment
173	Cq	3
140	Cq	7
128.4	CH	9/11
126.4	CH	10
126.1	CH	8/12
60.7	CH_2	2
26	CH	6
24	CH	4
17	CH_2	5
14	CH_3	1

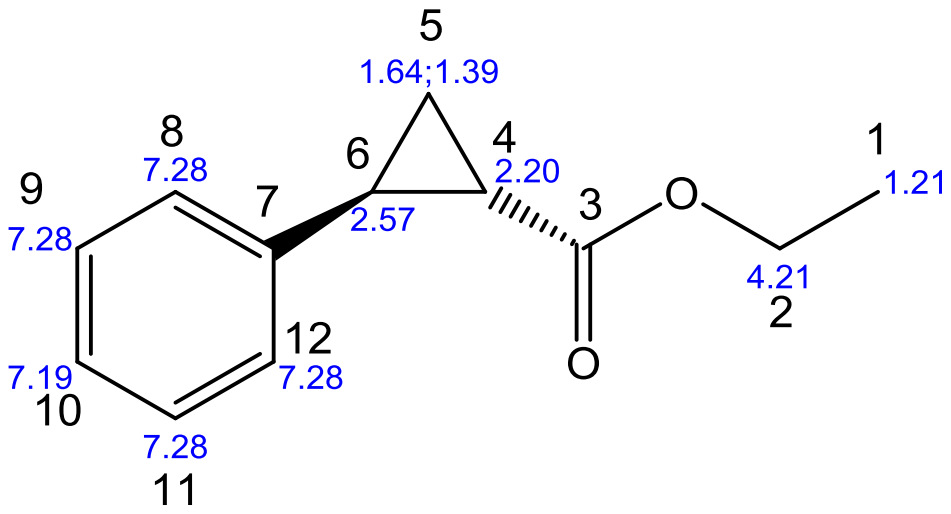
ChemNMR ^{13}C Estimation



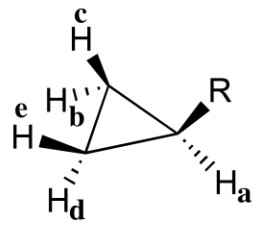
^{1}H-NMR/HSQC

δ (ppm)	integral	Signal	Assignment
7.3	2	multiplet (triplet-like)	9/11
7.2	1	multiplet (triplet-like)	10
7.1	2	multiplet (doublet-like)	8/12
4.2	2	Q	2
2.5	1	multiplet	6
1.9	1	multiplet	4
1.6	1	multiplet	5 (diastereotopic)
1.3	1	multiplet	
1.3	3	T	1

ChemNMR ^{1}H Estimation



^{1}H Chemical Shifts and Coupling Constants of Monosubstituted Cyclopropanes (δ in ppm, J in Hz)



	Substituent R	H_a	$H_{b;d}$	$H_{c;e}$	$^3J_{ab}$	$^3J_{ac}$	$^2J_{bc}$	$^3J_{bd}$	$^3J_{be}$	$^3J_{ce}$
	–H	0.20	0.20	0.20	9.0	5.6	-4.3	9.0	5.6	9.0
C	$–CH_3$	1.00	0.35	0.15						
	$–CH_2OH$	1.14	0.40	0.30						
	$–CH=CH_2$	1.35	0.64	0.34	8.2	4.9	-4.5	9.3	6.2	9.0
	–phenyl	1.83	0.89	0.65	9.5	6.3	-4.5	9.5	5.2	8.9
X	–F	4.32	0.69	0.27	5.9	2.4	-6.7	10.8	7.7	12.0
	–Cl	2.55	0.87	0.74	7.0	3.6	-6.0	10.3	7.1	10.6
	–Br	2.83	0.96	0.81	7.1	3.8	-6.1	10.2	7.0	10.5
	–I	2.31	1.04	0.76	7.5	4.4	-5.9	9.9	6.6	10.0
O	–OH	3.35	0.40	0.48	6.2	2.9	-5.4	10.3	6.8	10.9
N	$–NH_2$	2.23	0.32	0.20	6.6	3.6	-4.3	9.7	6.2	9.9
	$–NH_3^+$	1.06	0.52	0.34						
	$–NO_2$	4.21	1.13	1.60	7.0	3.4	-5.5	10.1	8.3	11.3
	–C≡N	1.29	0.96	1.04	8.4	5.1	-4.7	9.2	7.1	9.5
O	–CHO	1.79	0.99	1.03	8.0	4.6	-4.5	8.8	7.0	9.6
‖	$–COCH_3$	1.83	0.77	0.93	7.9	4.6	-3.5	9.2	7.0	9.5
C	–CO–cyclopropyl	1.70	0.56	1.02	7.9	4.6	-3.5	9.1	7.0	9.5
	–CO–phenyl	2.65	1.01	1.23						
	–COOH	1.59	0.91	1.05	8.0	4.6	-4.0	9.3	7.1	9.7
	$–COOCH_3$	1.61	0.86	0.98	8.0	4.6	-3.4	8.8	6.9	9.6
	$–CONH_2$	1.39	0.70	0.95						
	–COF	1.66	1.11	1.20	8.0	4.6	-4.5	10.1	7.5	9.3
	–COCl	2.11	1.18	1.28	7.9	4.4	-4.5	9.2	7.6	10.0