Table 3-8 Methyl and Methylene Groups

	δ(^{1}H)		δ(^{13}C)			δ(^{1}H)		δ(^{13}C)	
	CH_2	CH_3	CH_2	CH_3		CH_2	CH_3	CH_2	CH_3
CH_3Li		−0.4		−13.2	$(CH_3)_2NCHO$		2.88		36.0
CH_3CH_3		0.86		5.7			2.97		30.9
$(CH_3)_3CH$		0.89		25.2	CH_3Cl		3.06		25.1
$(CH_3)_4C$		0.94		31.7	$(CH_3)_2O$		3.24		59.5
$(CH_3)_3COH$		1.22		29.4	$(CH_3)_4N^+$		3.33		55.6
$CH_3CH{=}CH_2$		1.72		18.7	CH_3OH		3.38		49.2
$CH_3C{\equiv}CH$		1.80		−1.9	$CH_3CO_2CH_3$		3.67		51.0
$(CH_3)_3P{=}O$		1.93		18.6	$CH_3OC_6H_5$		3.73		54.8
CH_3CN		2.00		0.3	CH_3F		4.27		75.4
$CH_3CO_2CH_3$		2.01		18.7	CH_3NO_2		4.33		57.3
$CH_3(CO)CH_3$		2.07		30.2	$(CH_3CH_2)_2S$	2.49	1.25	26.5	15.8
CH_3CO_2H		2.10		18.6	$CH_3CH_2NH_2$	2.74	1.10	36.9	19.0
$(CH_3)_2S$		2.12		19.5	$CH_3CH_2C_6H_5$	2.92	1.18	29.3	16.8
CH_3I		2.15		−20.6	CH_3CH_2I	3.16	1.86	0.2	23.1
CH_3CHO		2.20		31.2	CH_3CH_2Br	3.37	1.65	28.3	20.3
$(CH_3)_3N$		2.22		47.3	CH_3CH_2Cl	3.47	1.33	39.9	18.7
$CH_3C_6H_5$		2.31		21.3	$(CH_3CH_2)_2O$	3.48	1.20	67.4	17.1
CH_3NH_2		2.42		30.4	CH_3CH_2OH	3.56	1.24	57.3	15.9
$CH_3(SO)CH_3$		2.50		40.1	CH_3CH_2F	4.36	1.24	79.3	14.6
$CH_3(CO)Cl$		2.67		32.7	$CH_3CH_2NO_2$	4.37	1.58	70.4	10.6
CH_3Br		2.69		10.2	$BrCH_2CH_2Br$	3.63		32.4	
$(CH_3)_4P^+$		2.74		11.3	$HOCH_2CH_2OH$	3.72		63.4	
$CH_3(SO_2)CH_3$		2.84		42.6	$ClCH_2CH_2Cl$	3.73		51.7	

Table 3-9 Saturated Ring Systems

		^{1}H	^{13}C			^{1}H	^{13}C
Cyclopropane		0.22	−2.6	Oxane (tetrahydropyran)	(α)	3.52	68.0
Cyclobutane		1.98	23.3		(β)	1.51	26.6
Cyclopentane		1.51	26.5		(γ)		23.6
Cyclohexane		1.43	27.7	Pyrrolidine	(α)	2.75	47.4
Cycloheptane		1.53	29.4		(β)	1.59	25.8
Cyclopentanone	(α)	2.06	37.0	Piperidine	(α)	2.74	47.5
	(β)	2.02	22.3		(β)	1.50	27.2
Cyclohexanone	(α)	2.22	40.7		(γ)	1.50	25.5
	(β)	1.8	26.8	Thiirane		2.27	18.9
	(γ)	1.8	24.1	Tetrahydrothiophene	(α)	2.82	31.7
Oxirane		2.54	40.5		(β)	1.93	31.2
Tetrahydrofuran	(α)	3.75	69.1	Sulfolane	(α)	3.00	51.1
	(β)	1.85	26.2		(β)	2.23	22.7
				1,4-Dioxane		3.70	66.5

Table 3-12 Carbonyl Compounds

	$^1H(CH_3)$	^1H(other)	$^{13}C(C{=}O)$
$H(CO)OCH_3$	3.79	8.05 (HCO)	160.9
$CH_3(CO)Cl$	2.67	—	168.6
$CH_3(CO)OCH_2CH_3$	2.02 (CH_3CO)	4.11 (CH_2), 1.24(CH_3C)	169.5
$CH_3(CO)N(CH_3)_2$	2.10 (CH_3CO)	6.94, 7.04 (CH_3N)	169.6
CH_3CO_2H	2.10	1.37 (HO)	177.3
$CH_3CO_2^-Na^+$	—	—	181.5
$CH_3(CO)C_6H_5$	2.62	—	196.0
$CH_3(CO)CH{=}CH_2$	2.32	5.8–6.4 ($CH{=}CH_2$)	197.2
$H(CO)CH_3$	2.20	9.80 (HCO)	199.6
$CH_3(CO)CH_3$	2.07	—	205.1
2-Cyclohexenone	—	5.93, 6.88 ($CH_\alpha{=}CH_\beta$)	197.1
2-Cyclopentanone	—	6.10, 7.71 ($CH_\alpha{=}CH_\beta$)	208.1
Cyclohexanone	—	1.7–2.5	208.8
Cyclopentanone	—	1.9–2.3	218.1

Table 3-10 Alkenes

		^{1}H	^{13}C
$CH_2{=}CHCN$	(α)	5.5–6.4	107.7
	(β)		137.8
$CH_2{=}CHC_6H_5$	(α)	6.66	112.3
	(β)	5.15, 5.63	135.8
$CH_2{=}CHBr$	(α)	6.4	115.6
	(β)	5.7–6.1	122.1
$CH_2{=}CHCO_2H$	(α)	6.5	128.0
	(β)	5.9–6.5	131.9
$CH_2{=}CH(CO)CH_3$	(α)	5.8–6.4	138.5
	(β)		129.3
$CH_2{=}CHO(CO)CH_3$	(α)	7.28	141.7
	(β)	4.56, 4.88	96.4
$CH_2{=}CHOCH_2CH_3$	(α)	6.45	152.9
	(β)	3.6–4.3	84.6
$CH_3\overset{4}{C}H{=}\overset{3}{C}CH_3{=}\overset{2}{C}H{=}\overset{1}{C}H_2$	(1)	5.02	
	(2)	6.40	
	(4)	5.70	

		^{1}H	^{13}C
$(CH_3)_2C{=}CHCO_2CH_3$	(α)	—	114.8
	(β)	5.62	155.9
Cyclopentene		5.60	130.6
Cyclohexene		5.59	127.2
1,3-Cyclopentadiene		6.42	132.2, 132.8
1,3-Cyclohexadiene		5.78	124.6, 126.1
2-Cyclopentenone	(α)	6.10	132.9
	(β)	7.71	164.2
2-Cyclohexenone	(α)	5.93	128.4
	(β)	6.88	149.8
exo-Methylenecyclohexane	($=CH_2$)	4.55	106.5
	(C=)	—	149.7
Allene	($=CH_2$)	4.67	74.0
	($=C=$)	—	213.0

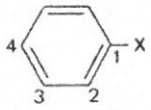
Table 3-11 Aromatics

	^{1}H			^{13}C			
	o	*m*	*p*	*i*	*o*	*m*	*p*
$C_6H_5CH_3$	7.16	7.16	7.16	137.8	129.3	128.5	125.6
$C_6H_5CH{=}CH_2$	7.24	7.24	7.24	138.2	126.7	128.9	128.2
$C_6H_5SCH_3$	7.23	7.23	7.23	138.7	126.7	128.9	124.9
C_6H_5F	6.97	7.25	7.05	163.8	114.6	130.3	124.3
C_6H_5Cl	7.29	7.21	7.23	135.1	128.9	129.7	126.7
C_6H_5Br	7.49	7.14	7.24	123.3	132.0	130.9	127.7
C_6H_5OH	6.77	7.13	6.87	155.6	116.1	130.5	120.8
$C_6H_5OCH_3$	6.84	7.18	6.90	158.9	113.2	128.7	119.8
$C_6H_5O(CO)CH_3$	7.06	7.25	7.25	151.7	122.3	130.0	126.4
$C_6H_5(CO)CH_3$	7.91	7.45	7.45	136.6	128.4	128.4	131.6
$C_6H_5CO_2H$	8.07	7.41	7.47	130.6	130.0	128.5	133.6
$C_6H_5(CO)Cl$	8.10	7.43	7.57	134.5	131.3	129.9	136.1
C_6H_5CN	7.54	7.38	7.57	109.7	130.1	127.2	130.1
$C_6H_5NH_2$	6.52	7.03	6.63	147.9	116.3	130.0	119.2
$C_6H_5NO_2$	8.22	7.48	7.61	148.3	123.4	129.5	134.7

	^{1}H			^{13}C		
	α	β	*Other*	α	β	*Other*
Naphthalene	7.81	7.46	—	128.3	126.1	—
Anthracene	7.91	7.39	8.31	130.3	125.7	132.8
Furan	7.40	6.30	—	142.8	109.8	—
Thiophene	7.19	7.04	—	125.6	127.4	—
Pyrrole	6.68	6.05	—	118.4	108.0	—
Pyridine	8.50	7.06	7.46	150.2	123.9	135.9

^{13}C-Chemical Shifts for Carbonyl Groups (δ in ppm relative to TMS)

R	R-CHO	R-$COCH_3$	R-COOH	R-COO^-	R-$COOCH_3$	R-$CONH_2$	R-COOCOR	R-COCl
-H		199.7	166.3	171.3	161.6	165.5		
-CH_3	199.7	206.0	178.1	181.7	170.7	172.7	167.3	168.6
-CH_2CH_3	201.8	207.6	180.4	185.1	173.3	177.2	170.3	174.7
-$CH(CH_3)_2$	204.0	211.8	184.1		175.7		172.8	178.0
-$C(CH_3)_3$		213.5	185.9	188.6	178.9	180.9	173.9	180.3
-n-C_8H_{17}	202.6	207.9	180.7	183.1	174.4	176.3	169.4	173.8
-CH_2Cl	193.3	200.7	173.8	174.7	167.8	168.3	162.1	167.7
-$CHCl_2$		193.6	170.3	170.6	165.1		157.6	165.5
-CCl_3	175.9	186.3	167.1		161.0		154.1	
-cyclohexyl	201.8	209.4	182.1	185.4	175.3			176.3
-$CH=CH_2$	192.4	197.2	171.7	179.3	165.5	168.3		165.6
-phenyl	192.0	197.6	172.6	175.6	166.8	169.7	162.8	168.0



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

	Substituent X	Z_1	Z_2	Z_3	Z_4
	-H	0.0	0.0	0.0	0.0
	$-CH_3$	9.3	0.6	0.0	-3.1
	$-CH_2CH_3$	15.7	-0.6	-0.1	-2.8
	$-CH(CH_3)_2$	20.1	-2.0	0.0	-2.5
	$-CH_2CH_2CH_2CH_3$	14.2	-0.2	-0.2	-2.8
	$-C(CH_3)_3$	22.1	-3.4	-0.4	-3.1
		15.1	-3.3	-0.6	-3.6
	$-CH_2Cl$	9.1	0.0	0.2	-0.2
	$-CH_2Br$	9.2	0.1	0.4	-0.3
C	$-CF_3$	2.6	-3.1	0.4	3.4
	$-CH_2OH$	13.0	-1.4	0.0	-1.2
		9.2	-3.1	-0.1	-0.5
	$-CH_2NH_2$	14.9	-1.6	-0.2	-2.0
	$-CH_2CN$	1.6	-0.7	0.5	-0.7
	$-CH=CH_2$	7.6	-1.8	-1.8	-3.5
	$-C\equiv CH$	-6.1	3.8	0.4	-0.2
	-phenyl	13.0	-1.1	0.5	-1.0
	-F	35.1	-14.3	0.9	-4.4
HAL	-Cl	6.4	0.2	1.0	-2.0
	-Br	-5.4	3.3	2.2	-1.0
	-I	-32.3	9.9	2.6	-0.4
	-OH	26.9	-12.7	1.4	-7.3
	$-O^-$	39.6	-8.2	1.9	-13.6
O	$-OCH_3$	30.2	-14.7	0.9	-8.1
	-Ophenyl	29.1	-9.5	0.3	-5.3
	$-OCOCH_3$	23.0	-6.4	1.3	-2.3
	$-NH_2$	19.2	-12.4	1.3	-9.5
	$-NHCH_3$	21.7	-16.2	0.7	-11.8
	$-N(CH_3)_2$	22.4	-15.7	0.8	-11.8
N	$-N(CH_2CH_3)_2$	19.3	-16.5	0.6	-13.0
	$-N(phenyl)_2$	19.3	-4.4	0.6	-5.9
	$-NHCOCH_3$	11.1	-9.9	0.2	-5.6
	$-NHNH_2$	22.8	-16.5	0.5	-9.6

	Substituent X	Z_1	Z_2	Z_3	Z_4
	-N=N-phenyl	24.0	-5.8	0.3	2.2
	$-N^+\equiv N$	-12.7	6.0	5.7	16.0
N	-NC	-1.8	-2.2	1.4	0.9
	-NCO	5.7	-3.6	1.2	-2.8
	-NO	37.4	-7.7	0.8	7.0
	$-NO_2$	19.6	-5.3	0.8	6.0
	-SH	2.2	0.7	0.4	-3.1
	$-SCH_3$	9.9	-2.0	0.1	-3.7
S	$-SC(CH_3)_3$	4.5	9.0	-0.3	0.0
	$-SO_2Cl$	15.6	-1.7	1.2	6.8
	$-SO_3H$	15.0	-2.2	1.3	3.8
	-CHO	9.0	1.2	1.2	6.0
	$-COCH_3$	9.3	0.2	0.2	4.2
O	-COOH	2.4	1.6	-0.1	4.8
‖	$-COO^-$	7.6	0.8	0.0	2.8
C	$-COOCH_3$	2.1	1.2	0.0	4.4
/	$-CONH_2$	5.4	-0.3	-0.9	5.0
\	-COCl	4.6	2.9	0.6	7.0
	-CN	-16.0	3.5	0.7	4.3
	$-P(phenyl)_2$ [1]	8.7	5.1	-0.1	0.0
	$-Si(CH_3)_3$	13.4	4.4	-1.1	-1.1

1) For ^{13}C-^{31}P-couplings see p. C245.

Table 4-1 One-Bond Couplings (Hz)

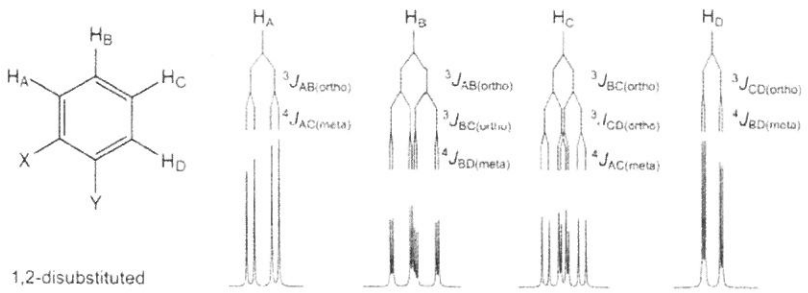
$^{13}C-^{1}H$	CH_3CH_3	125
	$(CH_3)_4Si$	118
	CH_3Li	98
	$(CH_3)_3N$	132
	CH_3CN	136
	$(CH_3)_2S$	138
	CH_3OH	142
	CH_3F	149
	CH_3Cl	150
	CH_2Cl_2	177
	$CHCl_3$	208
	Cyclohexane	125
	Cyclobutane	136
	Cyclopropane	162
	Tetrahydrofuran (α, β)	145, 133
	Norbornane (C1)	142
	Bicyclo[1.1.1]pentane (C1)	164
	Cyclohexene (C1)	157
	Cyclopropene (C1)	226
	Benzene	159
	1,3-Cyclopentadiene (C2)	170
	$CH_2=CHBr$ (gem)	197
	Acetaldehyde (CHO)	172
	Pyridine (α, β, γ)	177, 157, 160
	Allene	168
	Propyne (≡CH)	248
	$(CH_3)_2C^+H$ (^+CH)	164
	$HC\equiv N$	269
	Formaldehyde	222
	Formamide	191
$^{13}C-^{19}F$	CH_2F_2	235
	CF_3I	345
	C_6F_6	362
$^{13}C-^{31}P$	CH_3PH_2	9.3
	$(CH_3)_3P$	−13.6
	$(CH_3)_4P^+ I^-$	56
$^{13}C-^{15}N$	CH_3NH_2	−4.5
	$C_6H_5NH_2$	−11.4
	$CH_3(CO)NH_2$	−14.8
	$CH_3C\equiv N$	−17.5
	Pyridine	+0.62
	$CH_3HC=N-OH$ (*E*, *Z*)	−4.0, −2.3
$^{15}N-^{1}H$	CH_3NH_2	−64.5
	$CH_3(CO)NH_2$	−89
	Pyridinium	−90.5
	$HC\equiv N^+H$	−134
	$(C_6H_5)_2C=NH$	−51.2
$^{15}N-^{15}N$	Azoxybenzene	12.5
	Phenylhydrazine	6.7
$^{15}N-^{31}P$	$C_6H_5NHP(CH_3)_2$	53.0
	$C_6H_5NH(PO)(CH_3)_2$	−0.5
	$[(CH_3)_2N]_3P=O$	−26.9
$^{13}C-^{13}C$	CH_3CH_3	35
	$CH_3(CO)CH_3$	40
	CH_3CO_2H	57
	$CH_2=CH_2$	68
	$CH\equiv CH$	171
$^{31}P-^{1}H$	$C_6H_5(C_6H_5CH_2)(PO)H$	474
$^{31}P-^{31}P$	$(CH_3)_2P-P(CH_3)_2$	−179.7
	$(CH_3)_2(PS)(PS)(CH_3)_2$	18.7

Table 4-2 Geminal Proton–Proton (H—C—H) Couplings (Hz)

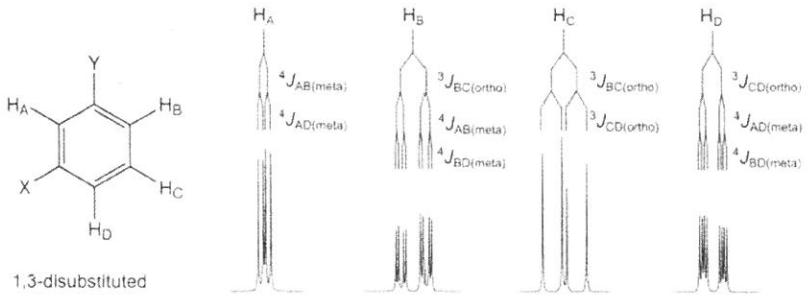
CH_4	−12.4	Oxirane	+5.5
$(CH_3)_4Si$	−14.1	$CH_2=CH_2$	+2.3
$C_6H_5CH_3$	−14.4	$CH_2=O$	+40.2
$CH_3(CO)CH_3$	−14.9	$CH_2=NOH$	9.9
CH_3CN	−16.9	$CH_2=CHF$	−3.2
$CH_2(CN)_2$	−20.4	$CH_2=CHNO_2$	−2.0
CH_3OH	−10.8	$CH_2=CHOCH_3$	−2.0
CH_3Cl	−10.8	$CH_2=CHBr$	−1.8
CH_3Br	−10.2	$CH_2=CHCl$	−1.4
CH_3F	−9.6	$CH_2=CHCH_3$	2.1
CH_3I	−9.2	$CH_2=CHCO_2H$	1.7
CH_2Cl_2	−7.5	$CH_2=CHC_6H_5$	1.1
Cyclohexane	−12.6	$CH_2=CHCN$	0.9
Cyclopropane	−4.3	$CH_2=CHLi$	7.1
Aziridine	+1.5	$CH_2=C=C(CH_3)_2$	−9.0

Table 4-3 Vicinal Proton–Proton (H—C—C—H) Couplings (Hz)

CH_3CH_3	8.0
$CH_3CH_2C_6H_5$	7.62
CH_3CH_2CN	7.60
CH_3CH_2Cl	7.23
$(CH_3CH_2)_3N$	7.13
CH_3CH_2OAc	7.12
$(CH_3CH_2)_2O$	6.97
CH_3CH_2Li	8.90
$(CH_3)_2CHCl$	6.4
$ClCH_2CH_2Cl$ (neat)	5.9
$Cl_2CHCHCl_2$ (neat)	3.06
Cyclopropane (cis, trans)	8.97, 5.58
Oxirane (cis, trans)	4.45, 3.10
Aziridine (cis, trans)	6.0, 3.1
Cyclobutane (cis, trans)	10.4, 4.9
Cyclopentane (cis, trans)	7.9, 6.3
Tetrahydrofuran (α–β: cis, trans)	7.94, 6.14
Cyclopentene (3–4: cis, trans)	9.36, 5.72
Cyclohexane (av.: cis, trans)	3.73, 8.07
Cyclohexane (ax–ax)	12.5
Cyclohexane (eq–eq and ax–eq)	3.7
Piperidine (av. α–β: cis, trans)	3.77, 7.88
Oxane (av. α–β: cis, trans)	3.87, 7.41
Cyclohexanone (av. α–β: cis, trans)	5.01, 8.61
Cyclohexene (3–4: (cis, trans)	2.95, 8.94
$CH_2=CH_2$ (cis, trans)	11.5, 19.0
$CH_2=CHLi$ (cis, trans)	19.3, 23.9
$CH_2=CHCN$ (cis, trans)	11.75, 17.92
$CH_2=CHC_6H_5$ (cis, trans)	11.48, 18.59
$CH_2=CHCO_2H$ (cis, trans)	10.2, 17.2
$CH_2=CHCH_3$ (cis, trans)	10.02, 16.81
$CH_2=CHCl$ (cis, trans)	7.4, 14.8
$CH_2=CHOCH_3$ (cis, trans)	7.0, 14.1
$ClHC=CHCl$ (cis, trans)	5.2, 12.2
Cyclopropene (1–2)	1.3
Cyclobutene (1–2)	2.85
Cyclopentene (1–2)	5.3
Cyclohexene (1–2)	8.8
Benzene	7.54
C_6H_5Li (2–3)	6.73
$C_6H_5CH_3$ (2–3)	7.64
$C_6H_5CO_2CH_3$ (2–3)	7.86
C_6H_5Cl (2–3)	8.05
$C_6H_5OCH_3$ (2–3)	8.30
$C_6H_5NO_2$ (2–3)	8.36
$C_6H_5N(CH_3)_2$ (2–3)	8.40
Naphthalene (1–2, 2–3)	8.28, 6.85
Furan (2–3, 3–4)	1.75, 3.3
Pyrrole (2–3, 3–4)	2.6, 3.4
Pyridine (2–3, 3–4)	4.88, 7.67

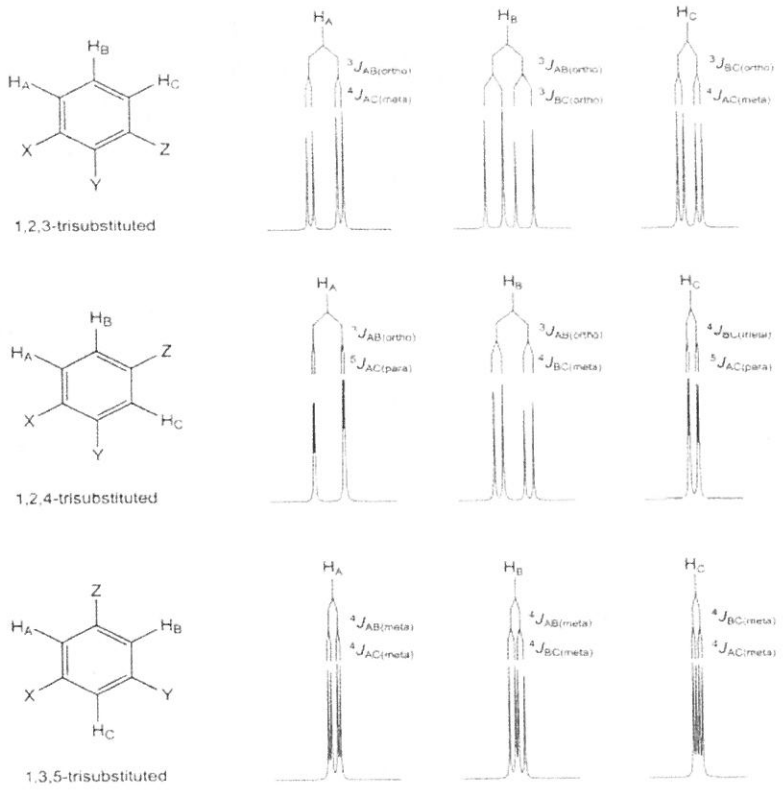


1,2-disubstituted



1,3-disubstituted

Characteristic aromatic splitting patterns in the ^{1}H NMR spectra of some disubstituted benzene rings.



1,2,3-trisubstituted

1,2,4-trisubstituted

1,3,5-trisubstituted

Characteristic aromatic splitting patterns in the ^{1}H NMR spectra for some trisubstituted benzenes.