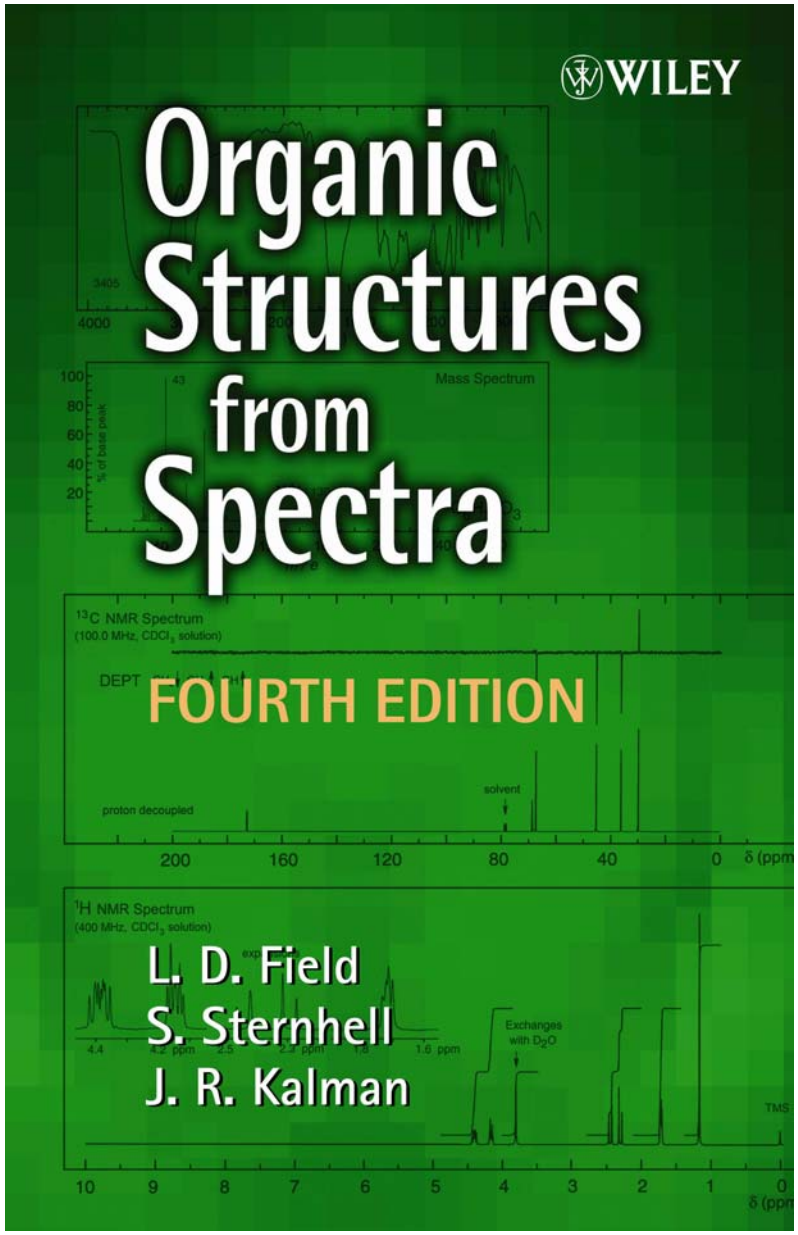
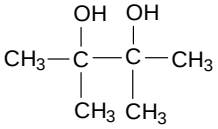
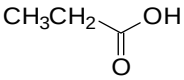
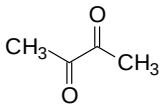
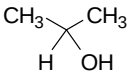
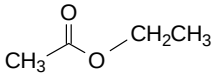
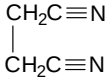
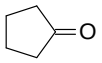
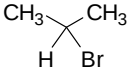
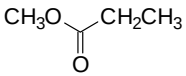
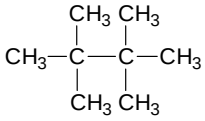
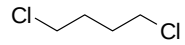
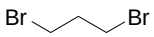
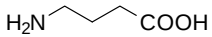
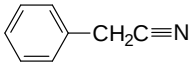
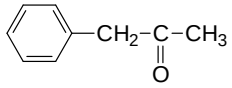
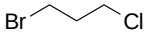
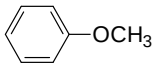
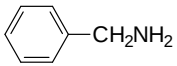
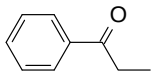
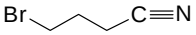
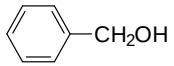
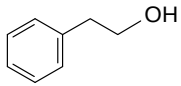
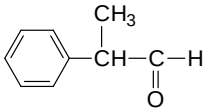
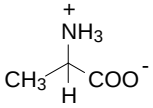
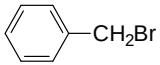
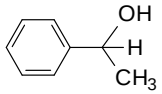
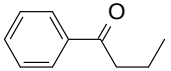


Solutions Manual

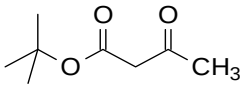
ORGANIC STRUCTURES FROM SPECTRA – 4th EDITION

L D Field, S Sternhell and J R Kalman

1  2-butanone C_4H_8O	**5** $BrCH_2-CH_2Br$ 1,2-dibromoethane $C_2H_4Br_2$	**9**  pinacol $C_6H_{14}O_2$	**13** Cl_2CH-CH_3 1,1-dichloroethane $C_2H_4Cl_2$
2  propionic acid $C_3H_6O_2$	**6**  1,2-butanedione (biacetyl) $C_4H_6O_2$	**10**  1,4-cyclohexanedione $C_6H_8O_2$	**14**  2-propanol C_3H_8O
3  ethyl acetate $C_4H_8O_2$	**7**  succinonitrile $C_4H_4N_2$	**11**  cyclopentanone $C_5H_8O_2$	**15**  2-bromopropane C_3H_7Br
4  methyl propionate $C_4H_8O_2$	**8**  2,2,3,3-tetramethylbutane C_8H_{18}	**12** CH_3CH_2-I iodoethane C_2H_5I	**16**  1,4-dichlorobutane $C_4H_8Cl_2$

17  1,3-dibromopropane $C_3H_6Br_2$	**21**  4-aminobutyric acid $C_4H_9NO_2$	**25**  benzyl cyanide C_8H_7N	**29**  benzyl methyl ketone $C_9H_{10}O$
18  1-bromo-3-chloropropane C_3H_6BrCl	**22**  anisole C_7H_8O	**26**  benzylamine C_7H_9N	**30**  propiophenone $C_9H_{10}O$
19  4-bromobutyronitrile C_4H_6NBr	**23**  benzyl alcohol C_7H_8O	**27**  2-phenylethanol $C_8H_{10}O$	**31**  2-phenylpropionaldehyde $C_9H_{10}O$
20  alanine $C_3H_7NO_2$	**24**  benzyl bromide C_7H_7Br	**28**  1-phenylethanol $C_8H_{10}O$	**32**  butyrophenone $C_{10}H_{12}O$

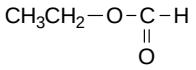
33



t-butyl acetoacetate

$C_8H_{14}O_3$

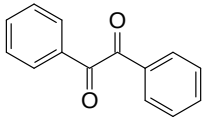
34



ethyl formate

$C_3H_6O_2$

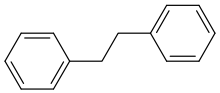
35



benzil

$C_{14}H_{10}O_2$

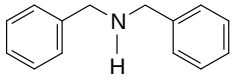
36



1,2-diphenylethane

$C_{14}H_{14}$

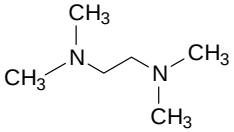
37



dibenzylamine

$C_{14}H_{15}N$

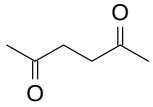
38



N,N,N,N-tetramethyl-1,2-ethanediamine

$C_6H_{16}N_2$

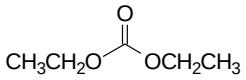
39



2,5-hexanedione

$C_6H_{10}O_2$

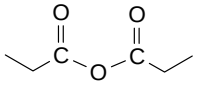
40



diethyl carbonate

$C_5H_{10}O_3$

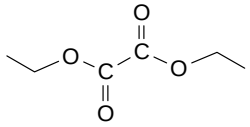
41



propionic anhydride

$C_6H_{10}O_3$

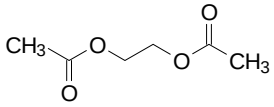
42



diethyl oxalate

$C_6H_{10}O_4$

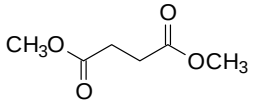
43



ethylene glycol diacetate

$C_6H_{10}O_4$

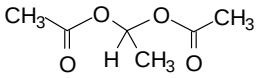
44



dimethyl succinate

$C_6H_{10}O_4$

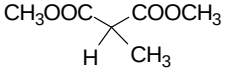
45



1,1-diacetoxyethane

$C_6H_{10}O_4$

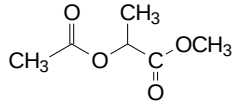
46



dimethyl methylmalonate

$C_6H_{10}O_4$

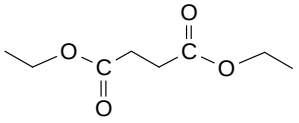
47



methyl acetyllactate

$C_6H_{10}O_4$

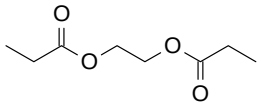
48



diethyl succinate

$C_8H_{14}O_4$

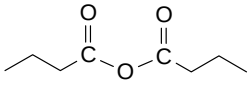
49



ethylene glycol dipropionate

$C_8H_{14}O_4$

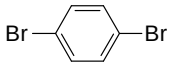
50



butyric anhydride

$C_8H_{14}O_3$

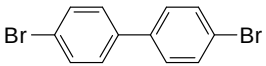
51



1,4-dibromobenzene

$C_6H_4Br_2$

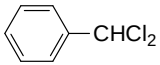
52



4,4'-dibromobiphenyl

$C_{12}H_8Br_2$

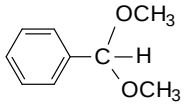
53



α,α-dichlorotoluene

$C_7H_6Cl_2$

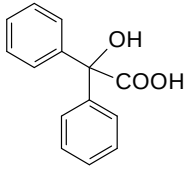
54



benzaldehyde dimethylacetal

$C_9H_{12}O_2$

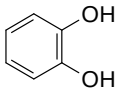
55



benzilic acid

$C_{14}H_{12}O_3$

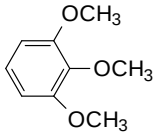
56



catechol

$C_6H_6O_2$

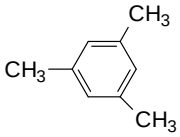
57



1,2,3-trimethoxybenzene

$C_9H_{12}O_3$

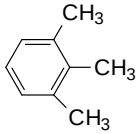
58



mesitylene

C_9H_{12}

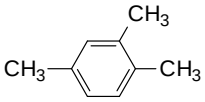
59



1,2,3-trimethylbenzene

C_9H_{12}

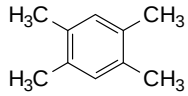
60



1,2,4-trimethylbenzene

C_9H_{12}

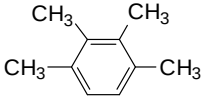
61



durene

$C_{10}H_{14}$

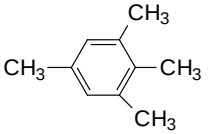
62



1,2,3,4-tetramethylbenzene

$C_{10}H_{14}$

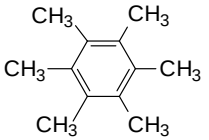
63



1,2,3,5-tetramethylbenzene

$C_{10}H_{14}$

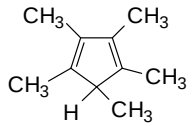
64



hexamethylbenzene

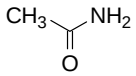
$C_{12}H_{18}$

65



1,2,3,4,5,-pentamethylcyclopentadiene
$C_{10}H_{16}$

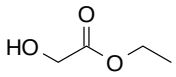
66



acetamide

C_2H_5NO

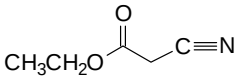
67



ethyl glycolate

$C_4H_8O_3$

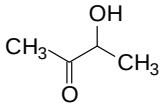
68



ethyl cyanoacetate

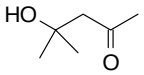
$C_5H_7NO_2$

69



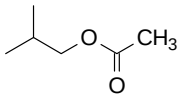
3-hydroxybutanone
(acetoin)
$C_4H_8O_2$

70



4-hydroxy-4-methyl-2-pentanone
$C_6H_{12}O_2$

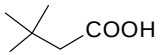
71



isobutyl acetate

$C_6H_{12}O_2$

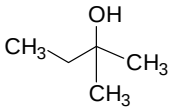
72



3,3-dimethylbutyric acid

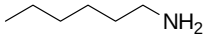
$C_6H_{12}O_2$

73



2-methyl-2-butanol
(*t*-amyl alcohol)
$C_5H_{12}O$

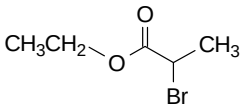
74



hexylamine

$C_6H_{15}N$

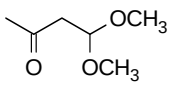
75



ethyl 2-bromopropionate

$C_5H_9O_2Br$

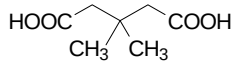
76



4,4-dimethoxy-2-butanone

$C_6H_{12}O_3$

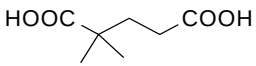
77



3,3-dimethylglutaric acid

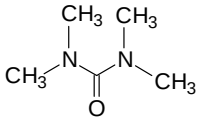
$C_7H_{12}O_4$

78



2,2-dimethylpentanedioc acid
$C_7H_{12}O_4$

79



tetramethylurea

$C_5H_{12}N_2O$

80

1,3-dioxan

$C_4H_8O_2$

ORGANIC STRUCTURES FROM SPECTRA – 4th EDITION

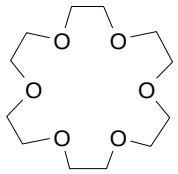
L D Field, S Sternhell and J R Kalman

81

1,4-dioxan

$C_4H_8O_2$

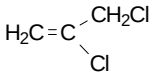
82



18-crown-6

$C_{12}H_{24}O_6$

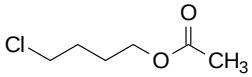
83



2,3-dichloropropene

$C_3H_4Cl_2$

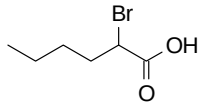
84



4-chlorobutyl acetate

$C_6H_{11}O_2Cl$

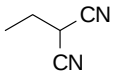
85



2-bromohexanoic acid

$C_6H_{11}O_2Br$

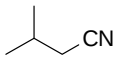
86



2-ethylmalononitrile

$C_5H_6N_2$

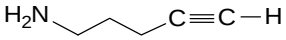
87



3-methylbutyronitrile

C_5H_9N

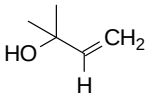
88



5-amino-1-pentyne

C_5H_9N

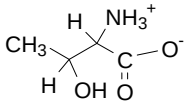
89



2-methylbut-3-en-2-ol

$C_5H_{10}O$

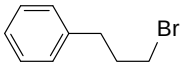
90



threonine

$C_4H_9NO_3$

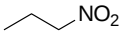
91



1-bromo-3-phenylpropane

$C_9H_{11}Br$

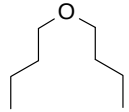
92



1-nitropropane

$C_3H_7NO_2$

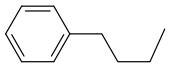
93



dibutyl ether

$C_8H_{18}O$

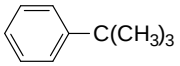
94



butylbenzene

$C_{10}H_{14}$

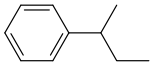
95



t-butylbenzene

$C_{10}H_{14}$

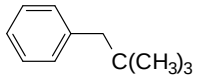
96



sec-butylbenzene

$C_{10}H_{14}$

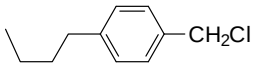
97



neopentylbenzene

$C_{11}H_{16}$

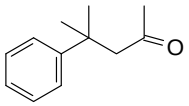
98



4-(*n*-butyl)-α-chlorotoluene

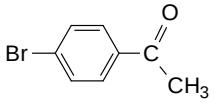
$C_{11}H_{15}Cl$

99



4-methyl-4-phenyl-2-pentanone
$C_{12}H_{16}O$

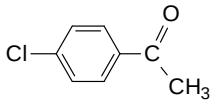
100



p-bromoacetophenone

C_8H_7OBr

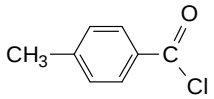
101



p-chloroacetophenone

C_8H_7OCl

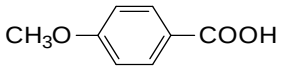
102



p-toluyl chloride

C_8H_7OCl

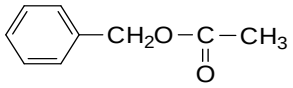
103



p-anisic acid

$C_8H_8O_3$

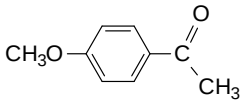
104



benzyl acetate

$C_9H_{10}O_2$

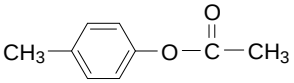
105



4-methoxyacetophenone

$C_9H_{10}O_2$

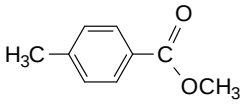
106



p-cresyl acetate

$C_9H_{10}O_2$

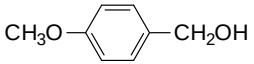
107



methyl *p*-toluate

$C_9H_{10}O_2$

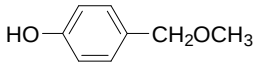
108



p-methoxybenzyl alcohol

$C_8H_{10}O_2$

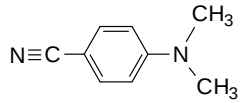
109



4-methoxymethylphenol

$C_8H_{10}O_2$

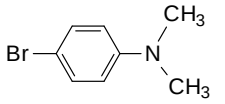
110



4-dimethylaminobenzonitrile

$C_9H_{10}N_2$

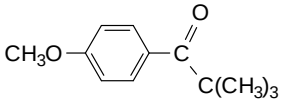
111



p-bromo-*N*,*N*-dimethylaniline

$C_8H_{10}NBr$

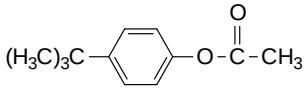
112



p-anisyl *t*-butyl ketone

$C_{12}H_{16}O_2$

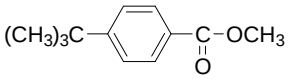
113



4-*t*-butylphenyl acetate

$C_{12}H_{16}O_2$

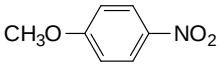
114



methyl 4-*t*-butylbenzoate

$C_{12}H_{16}O_2$

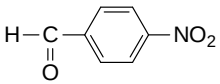
115



p-nitroanisole

$C_7H_7NO_3$

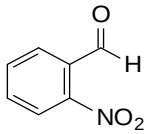
116



p-nitrobenzaldehyde

$C_7H_5NO_3$

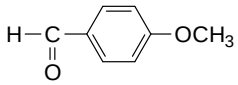
117



o-nitrobenzaldehyde

$C_7H_5NO_3$

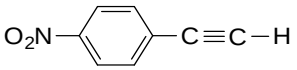
118



4-methoxybenzaldehyde

$C_8H_8O_2$

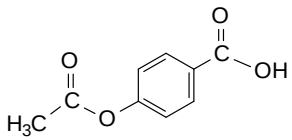
119



4-nitrophenylacetylene

$C_8H_5NO_2$

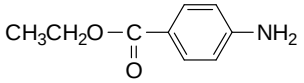
120



4-acetoxybenzoic acid

$C_9H_8O_4$

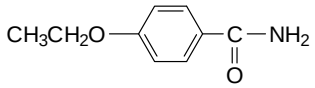
121



ethyl *p*-aminobenzoate

$C_9H_{11}NO_2$

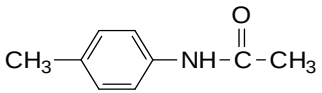
122



p-ethoxybenzamide

$C_9H_{11}NO_2$

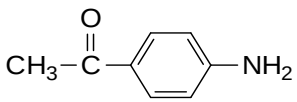
123



4-methylacetanilide

C_8H_9NO

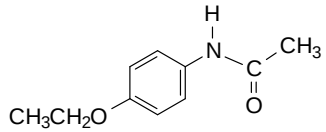
124



4-aminoacetophenone

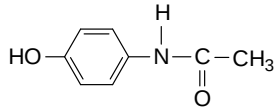
C_8H_9NO

125



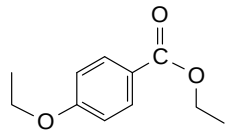
p-ethoxyacetanilide
(phenacetin)
$C_{10}H_{13}NO_2$

126



p-hydroxyacetanilide
(paracetamol)
$C_8H_9NO_2$

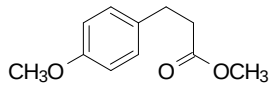
127



ethyl *p*-ethoxybenzoate

$C_{11}H_{14}O_3$

128

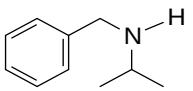


methyl (*p*-methoxyphenyl)-
propionionate
$C_{11}H_{14}O_3$

ORGANIC STRUCTURES FROM SPECTRA – 4th EDITION

L D Field, S Sternhell and J R Kalman

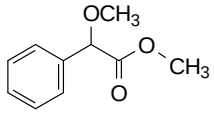
129



N-isopropylbenzylamine

$C_{10}H_{15}N$

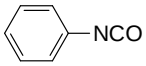
130



methyl 2-methoxy-2-phenylacetate

$C_{10}H_{12}O_3$

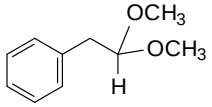
131



phenyl isocyanate

C_7H_5NO

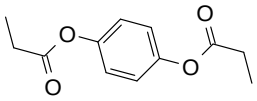
132



phenylacetaldehyde dimethyl acetal

$C_{10}H_{14}O_2$

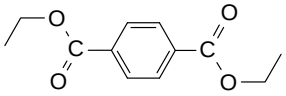
133



hydroquinone dipropionate

$C_{12}H_{14}O_4$

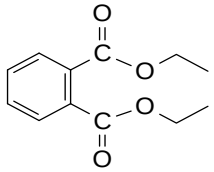
134



diethyl terephthalate

$C_{12}H_{14}O_4$

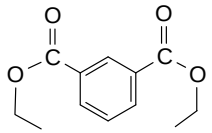
135



diethyl *o*-phthalate

$C_{12}H_{14}O_4$

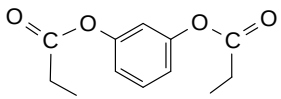
136



diethyl isophthalate

$C_{12}H_{14}O_4$

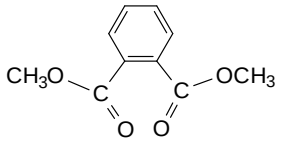
137



1,3-dihydroxyphenyl dipropionate

$C_{12}H_{14}O_4$

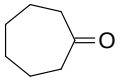
138



dimethyl *o*-phthalate

$C_{10}H_{10}O_4$

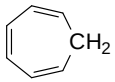
139



cycloheptanone

$C_7H_{12}O$

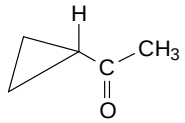
140



cycloheptatriene

C_7H_8

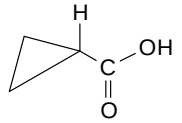
141



cyclopropyl methyl ketone

C_5H_8O

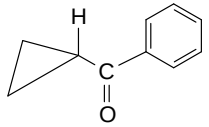
142



cyclopropane carboxylic acid

$C_4H_6O_2$

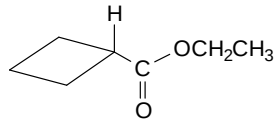
143



benzoylcylopropane

$C_{10}H_{10}O$

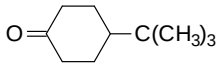
144



ethyl cyclobutanecarboxylate

$C_7H_{12}O_2$

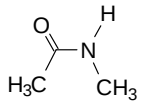
145



4-*t*-butylcyclohexanone

$C_{10}H_{18}O$

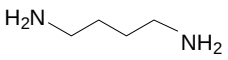
146



N-methylacetamide

C_3H_7NO

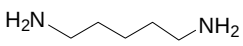
147



1,4-diaminobutane

$C_4H_{12}N_2$

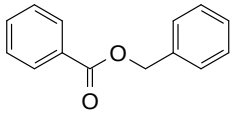
148



1,5-diaminopentane

$C_5H_{14}N_2$

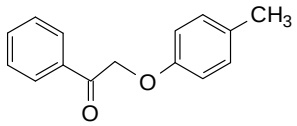
149



benzyl benzoate

$C_{14}H_{12}O_2$

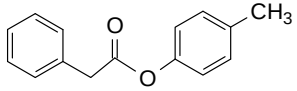
150



(*p*-cresyl)methyl phenyl ketone

$C_{15}H_{14}O_2$

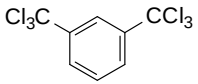
151



p-cresyl phenylacetate

$C_{15}H_{14}O_2$

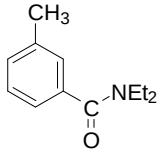
152



1,3-bis(trichloromethyl)-benzene

$C_8H_4Cl_6$

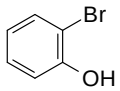
153



N,N-diethyl-*m*-toluamide

$C_{12}H_{17}NO$

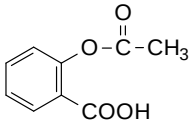
154



2-bromophenol

C_6H_5OBr

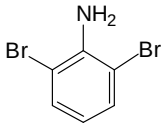
155



acetylsalicylic acid (aspirin)

$C_9H_8O_4$

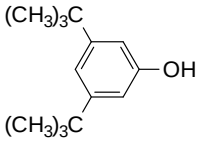
156



2,6-dibromoaniline

$C_6H_5NBr_2$

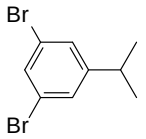
157



3,5-di-*t*-butylphenol

$C_{14}H_{22}O$

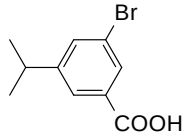
158



3,5-dibromocumene

$C_9H_{10}Br_2$

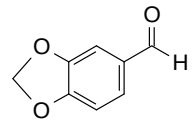
159



3-bromo-5-isopropylbenzoic acid

$C_{10}H_{11}O_2Br$

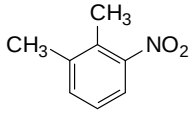
160



piperonal

$C_8H_6O_3$

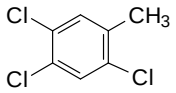
161



3-nitro-*o*-xylene

$C_8H_9NO_2$

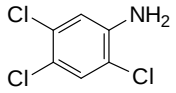
162



2,4,5-trichlorotoluene

$C_7H_5Cl_3$

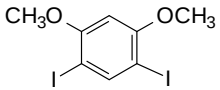
163



2,4,5-trichloroaniline

$C_6H_4NCl_3$

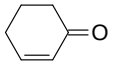
164



4,6-diiodo-1,3-dimethoxybenzene

$C_8H_8O_2I_2$

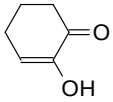
165



2-cyclohexene-1-one

C_6H_8O

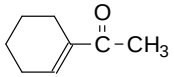
166



2-hydroxycyclohex-1-en-3-one

$C_6H_8O_2$

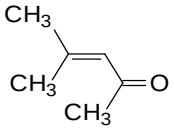
167



1-acetyl-1-cylohexene

$C_8H_{12}O$

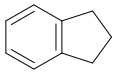
168



4-methylpent-3-en-2-one (mesityl oxide)

$C_6H_{10}O$

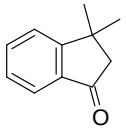
169



indane

C_9H_{10}

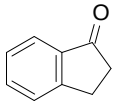
170



3,3-dimethylindan-1-one

$C_{11}H_{12}O$

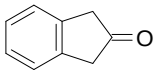
171



1-indanone

C_9H_8O

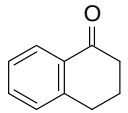
172



2-indanone

C_9H_8O

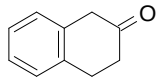
173



α-tetralone

$C_{10}H_{10}O$

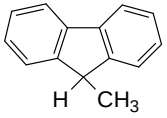
174



β-tetralone

$C_{10}H_{10}O$

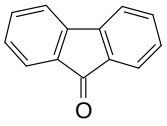
175



9-methylfluorene

$C_{14}H_{12}$

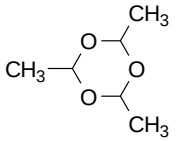
176



fluorenone

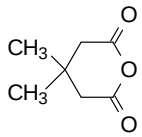
$C_{13}H_8O$

177



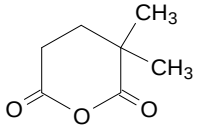
2,4,6-trimethyl-1,3,5-trioxane
$C_6H_{12}O_3$

178



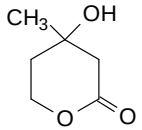
3,3-dimethylglutaric anhydride
$C_7H_{10}O_3$

179



2,2-dimethylglutaric anhydride
$C_7H_{10}O_3$

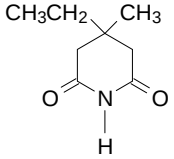
180



mevalonic lactone

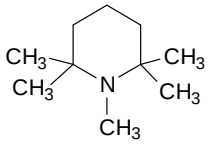
$C_6H_{10}O_3$

181



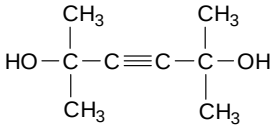
4-ethyl-4-methyl-2,6-piperidinedione
$C_8H_{13}NO_2$

182



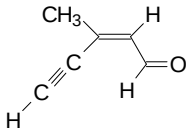
1,2,2,6,6-pentamethyl-piperidine
$C_{10}H_{21}N$

183



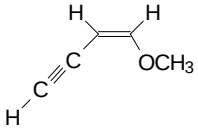
2,5-dimethyl-3-hexyne-2,5-diol
$C_8H_{14}O_2$

184



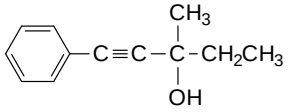
(*Z*)-3-methylpent-2-en-4-ynal
C_6H_6O

185



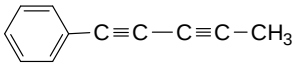
(*Z*)-1-methoxybut-1-en-4-yne
C_5H_6O

186



3-methyl-1-phenylpent-1-yn-3-ol
$C_{12}H_{14}O$

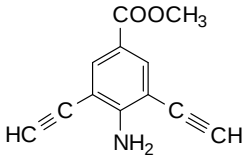
187



1-phenyl-1,3-pentadiyne

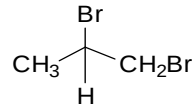
$C_{11}H_8$

188



methyl 4-amino-3,5-diethynylbenzoate
$C_{12}H_9NO_2$

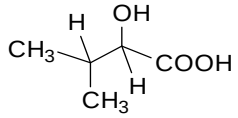
189



1,2-dibromopropane

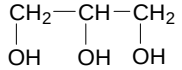
$C_3H_6Br_2$

190



2-hydroxy-3-methylbutyric acid
$C_5H_{10}O_3$

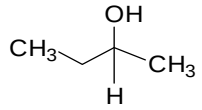
191



glycerol

$C_3H_8O_3$

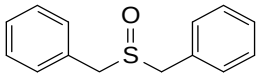
192



2-butanol

$C_4H_{10}O$

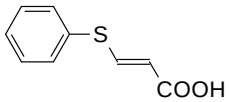
193



dibenzyl sulfoxide

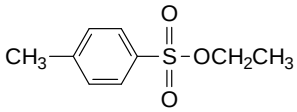
$C_{14}H_{14}OS$

194



(*E*)-3-(phenylthio)acrylic acid
$C_9H_8O_2S$

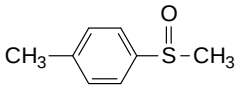
195



ethyl *p*-toluenesulfonate

$C_9H_{12}O_3S$

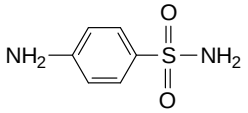
196



p-tolyl methyl sulfoxide

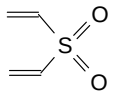
$C_8H_{10}OS$

197



p-amino-benzenesulfonamide
$C_6H_8N_2O_2S$

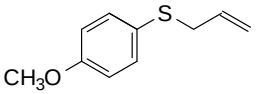
198



divinyl sulfone

$C_4H_6O_2S$

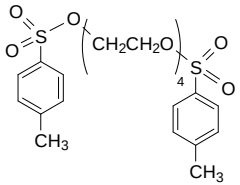
199



allyl *p*-anisyl thioether

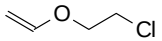
$C_{10}H_{12}OS$

200



tetraethylene glycol ditosylate
$C_{22}H_{30}O_9S_2$

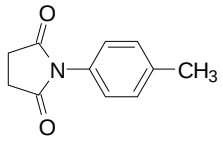
201



vinyl 2-chloroethyl ether

C_4H_7OCl

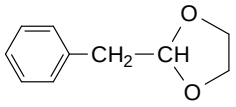
202



N-(*p*-tolyl)succinimide

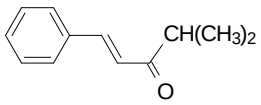
$C_{11}H_{11}NO_2$

203



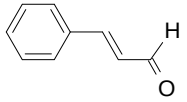
phenylacetaldeyde ethylene glycol acetal
$C_{10}H_{12}O_2$

204



(*E*)-1-phenyl-4-methyl-1-penten-3-one
$C_{12}H_{14}O$

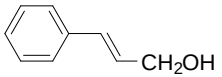
205



cinnamaldehyde

C_9H_8O

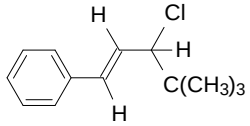
206



cinnamyl alcohol

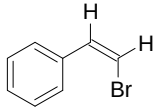
$C_9H_{10}O$

207



(*E*)-3-chloro-4,4-dimethyl-1-phenyl-1-pentene
$C_{13}H_{17}Cl$

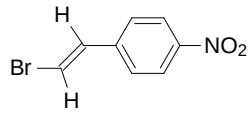
208



(*Z*)-β-bromostyrene

C_8H_7Br

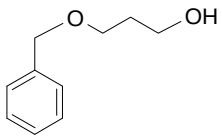
209



(E)-*p*-nitro-β-bromostyrene

$C_8H_6BrNO_2$

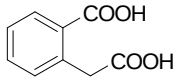
210



3-benzyloxy-1-propanol

$C_{10}H_{14}O_2$

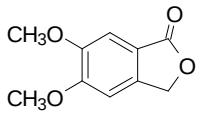
211



homophthallic acid

$C_9H_8O_4$

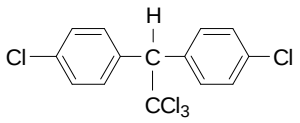
212



5,6-dimethoxy-2-coumaranone

$C_{10}H_{10}O_4$

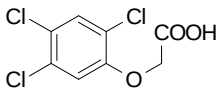
213



1,1-di-(*p*-chlorophenyl)-2,2,2-trichloroethane (DDT)

$C_{14}H_9Cl_5$

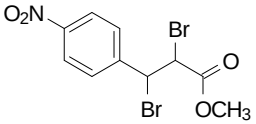
214



2,4,5-trichlorophenoxy-acetic acid (2,4,5-T)

$C_8H_5O_3Cl_3$

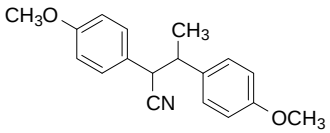
215



methyl 2,3-dibromo-3-(*p*-nitrophenyl)propionate

$C_{10}H_9NO_4Br_2$

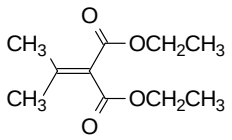
216



2,3-di-(*p*-anisyl)butyronitrile

$C_{18}H_{19}NO_2$

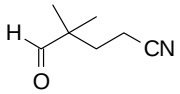
217



diethyl isopropylidene-malonate

$C_{10}H_{16}O_4$

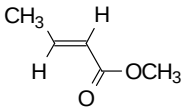
218



4-cyano-2,2-dimethylbutyraldehyde

$C_7H_{11}NO$

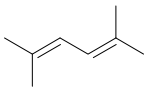
219



methyl (*E*)-3-methylacrylate

$C_5H_8O_2$

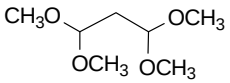
220



2,5-dimethyl-2,4-hexadiene

C_8H_{14}

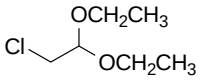
221



malonaldehyde dimethyl acetal

$C_7H_{16}O_4$

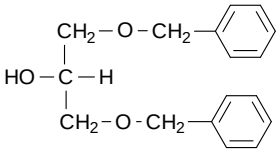
222



2-chloroacetaldehyde diethylacetal

$C_6H_{13}O_2Cl$

223



1,3-dibenzylglycerol

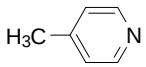
$C_{17}H_{20}O_3$

224

pyridine

C_5H_5N

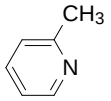
225



4-picoline

C_6H_7N

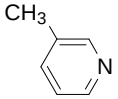
226



2-picoline

C_6H_7N

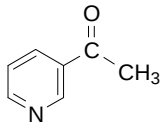
227



3-picoline

C_6H_7N

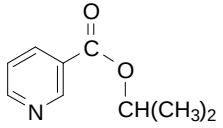
228



3-acetylpyridine

C_7H_7NO

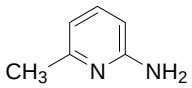
229



isopropyl nicotinate

$C_9H_{11}NO_2$

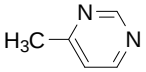
230



2-methyl-6-aminopyridine

$C_6H_8N_2$

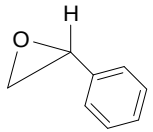
231



4-methylpyrimidine

$C_5H_6N_2$

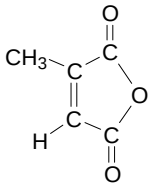
232



styrene epoxide

C_8H_8O

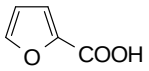
233



citraconic anhydride

$C_5H_4O_3$

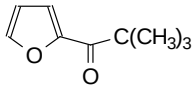
234



2-furoic acid

$C_5H_4O_3$

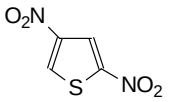
235



2-furyl *t*-butyl ketone

$C_9H_{12}O_2$

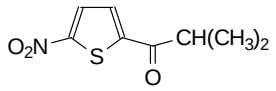
236



2,4-dinitrothiophene

$C_4H_2N_2O_4S$

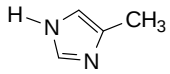
237



2-(5-nitrothienyl) isopropyl ketone

$C_8H_9NO_3S$

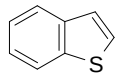
238



4-methylimidazole

$C_4H_6N_2$

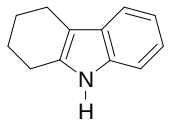
239



benzothiophene

C_8H_6S

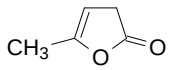
240



2,3,4,9-tetrahydrocarbazole

$C_{12}H_{13}N$

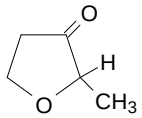
241



α-angelicalactone

$C_5H_6O_2$

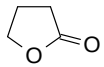
242



2-methyl-tetrahydrofuran-3-one

$C_5H_8O_2$

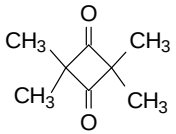
243



butyrolactone

$C_4H_6O_2$

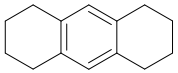
244



tetramethyl-1,3-cyclobutanedione

$C_8H_{12}O_2$

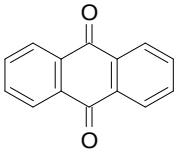
245



octahydroanthracene

$C_{14}H_{18}$

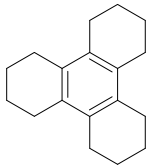
246



anthraquinone

$C_{14}H_8O_2$

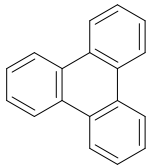
247



dodecahydrotriphenylene

$C_{18}H_{24}$

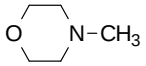
248



triphenylene

$C_{18}H_{12}$

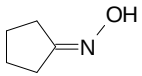
249



N-methylmorpholine

$C_5H_{11}NO$

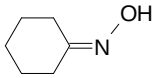
250



cyclopentanone oxime

C_5H_9NO

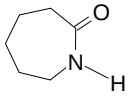
251



cyclohexanone oxime

$C_6H_{11}NO$

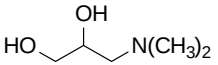
252



ε-caprolactam

$C_6H_{11}NO$

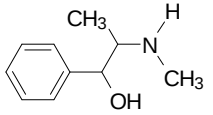
253



N,N-dimethyl-2,3-dihydroxy-1-propylamine

$C_5H_{13}NO_2$

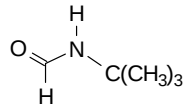
254



pseudoephedrine

$C_{10}H_{15}NO$

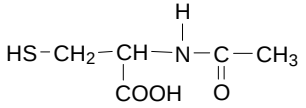
255



t-butylformamide

$C_5H_{11}NO$

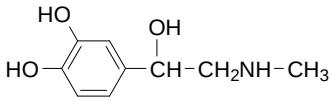
256



N-acetylcysteine

$C_5H_9NO_3S$

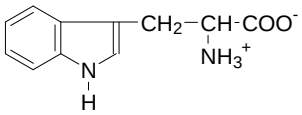
257



adrenalin

$C_9H_{13}NO_3$

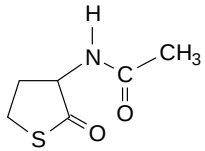
258



tryptophan

$C_{11}H_{12}N_2O_2$

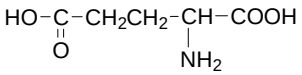
259



N-acetylhomocysteine thiolactone

$C_6H_9NO_2S$

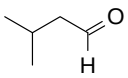
260



glutamic acid

$C_5H_9NO_4$

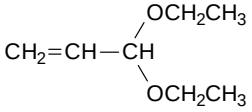
261



3-methylbutyraldehyde

$C_5H_{10}O$

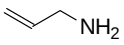
262



acrolein diethyl acetal

$C_7H_{14}O_2$

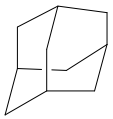
263



allylamine

C_3H_7N

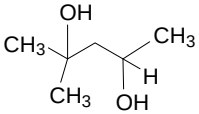
264



adamantine

$C_{10}H_{16}$

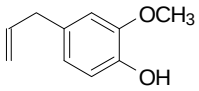
265



2-methyl-2,4-pentanediol

$C_6H_{14}O_2$

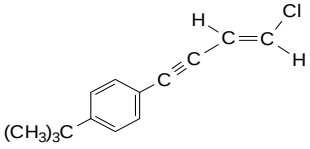
266



eugenol

$C_{10}H_{12}O_2$

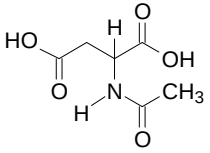
267



E -1-chloro-4-(4-*t*-butylphenyl)but-1-en-3-yne

$C_{14}H_{15}Cl$

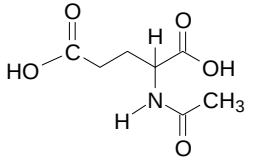
268



N-acetylaspartic acid

$C_6H_9NO_5$

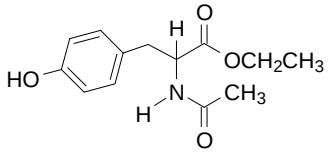
269



N-acetylglutamic acid

$C_7H_{11}NO_5$

270



N-acetyltyrosine ethyl ester

$C_{13}H_{17}NO_4$

271

2,5-dihydrofuran

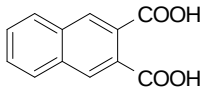
C_4H_6O

272

2,3-dihydrofuran

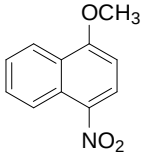
C_4H_6O

273



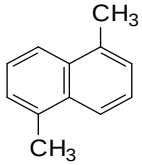
2,3-naphthalene-dicarboxylic acid
$C_{12}H_8O_4$

274



1-methoxy-4-nitro-naphthalene
$C_{11}H_9NO_3$

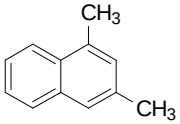
275



1,5-dimethylnaphthalene

$C_{12}H_{12}$

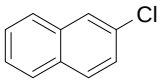
276



1,3-dimethylnaphthalene

$C_{12}H_{12}$

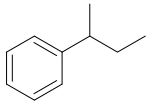
277



2-chloronaphthalene

$C_{10}H_7Cl$

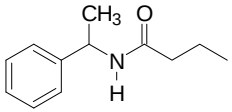
278



sec-butylbenzene

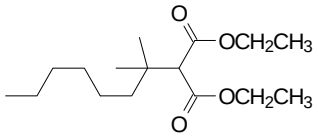
$C_{10}H_{14}$

279



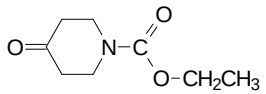
N-(1-methyl-1-phenylethyl)-butyramide
$C_{12}H_{17}NO$

280



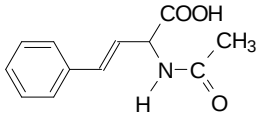
diethyl 2-(1,1-dimethylheptyl)malonate
$C_{16}H_{30}O_4$

281



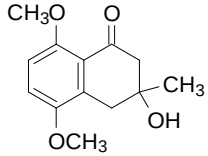
ethyl 4-piperidone-*N*-carboxylate
$C_8H_{13}NO_3$

282



N-acetyl-2-amino-4-phenyl-(*E*)-but-2-enoic acid
$C_{12}H_{13}NO_3$

283



3-hydroxy-3-methyl-5,8-dimethoxy-1-coumarinone
$C_{13}H_{16}O_4$

Chapter 9.2 – The Analysis of MixturesProblem 284

Problem 284

Compound	Mole %
ethanol	57
bromoethane	43

Problem 285

Compound	Mole %
benzene	15
diethyl ether	46
dichoromethane	39

Problem 286

Compound	Mole %
benzene	24
ethyl acetate	59
dioxane	17

Problem 287

Compound	Mole %
ethanol	41
bromoethane	59

Problem 288

Compound	Mole %
benzene	13
diethyl ether	22
dichoromethane	65

Problem 289

Compound	Mole %
benzene	23
ethyl acetate	51
dioxane	26

Problem 290

Compound	Mole %
fluorene	75
fluorenone	25

Problem 291

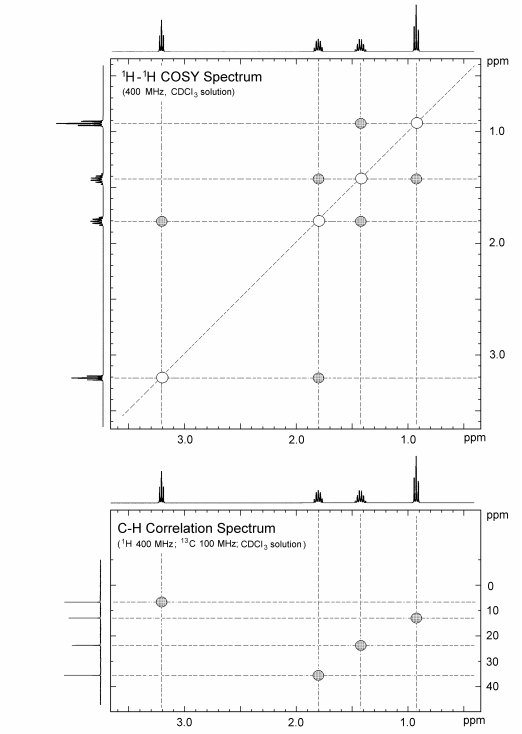
Compound	Mole %
4-nitroanisole	38
2-nitroanisole	62

Chapter 9.3 – Problems in 2D NMR

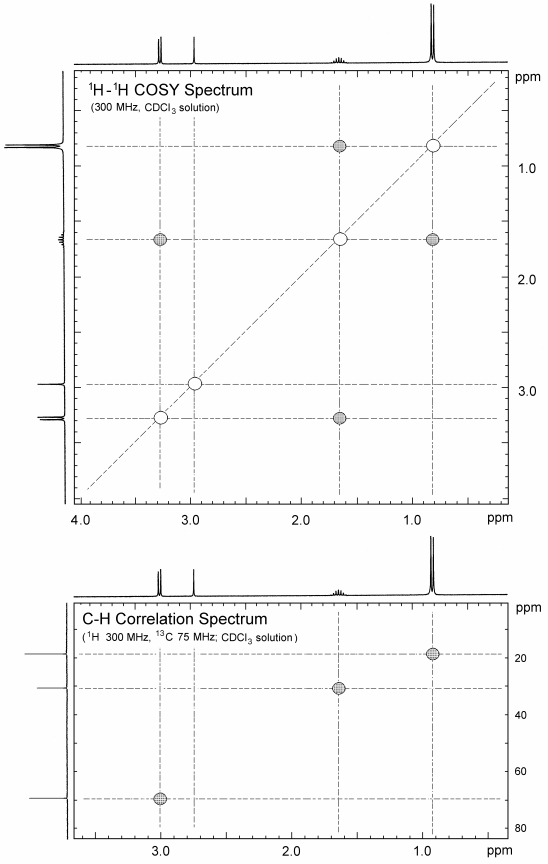
Problem 292 1-propanol

Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
H1	3.49	**C1**	64.0
H2	1.50	**C2**	25.5
H3	0.85	**C3**	9.9
H4	2.95		

Problem 293 1-iodobutane

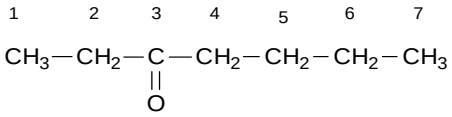


Problem 294 isobutanol



Problem 295

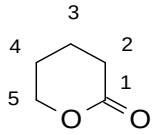
3-heptanone



Proton	Chemical Shift (δ) in ppm
H1	0.91
H2	1.94
H4	1.97
H5	1.44
H6	1.14
H7	0.79

Problem 296

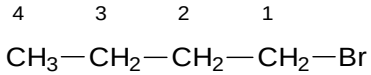
δ-valerolactone



Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
		C1	170.0
H2	2.08	**C2**	29.9
H3	1.16	**C3**	22.2
H4	1.08	**C4**	19.0
H5	3.71	**C5**	68.8

Problem 297

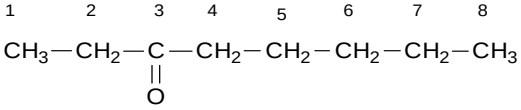
1-bromobutane



Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
H1	3.39	**C1**	33.4
H2	1.82	**C2**	34.7
H3	1.45	**C3**	21.4
H4	0.91	**C4**	13.2

Problem 298

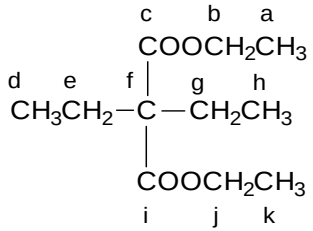
3-octanone



Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
H1	0.92	**C1**	7.8
H2	1.92	**C2**	35.4
		C3	209.0
H4	1.94	**C4**	42.1
H5	1.47	**C5**	23.7
H6	1.11	**C6**	31.7
H7	1.19	**C7**	22.7
H8	0.82	**C8**	14.0

Problem 299

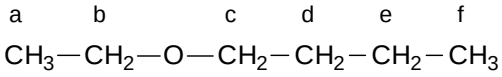
diethyl diethylmalonate



Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
H_a	1.19	C_a	14.0
H_b	4.13	C_b	60.8
		C_c	171.9
H_d	0.76	C_d	8.1
H_e	1.88	C_e	24.5
		C_f	58.0
H_g	1.88	C_g	24.5
H_h	0.76	C_h	8.1
		C_i	171.9
H_j	4.13	C_j	60.8
H_k	1.19	C_k	14.0

Problem 300

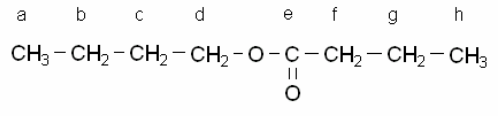
butyl ethyl ether



Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
H_a	1.11	C_a	15.0
H_b	3.29	C_b	66.0
H_c	3.27	C_c	70.1
H_d	1.52	C_d	32.1
H_e	1.36	C_e	19.4
H_f	0.87	C_f	13.5

Problem 301

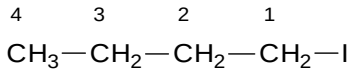
butyl butyrate



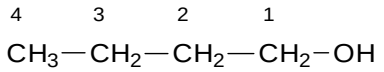
Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
H_a	0.75	C_a	13.9
H_b	1.19	C_b	19.5
H_c	1.40	C_c	31.2
H_d	3.97	C_d	64.0
		C_e	172.8
H_f	2.08	C_f	36.2
H_g	1.52	C_g	19.0
H_h	0.79	C_h	13.9

Problem 302

1-iodobutane



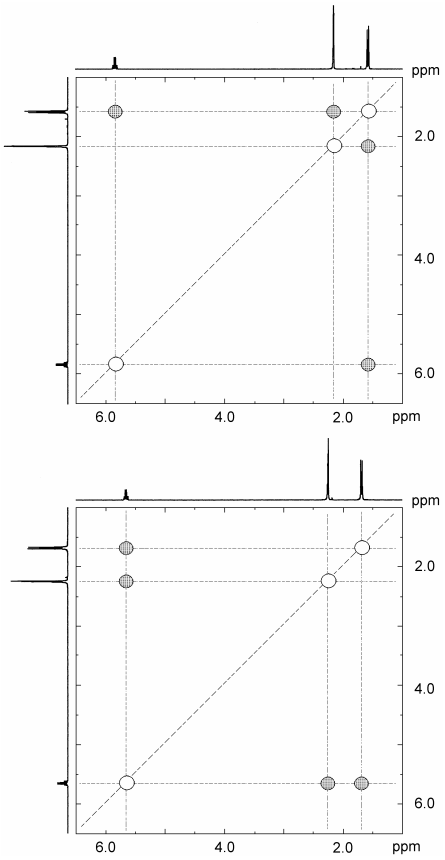
1-butanol

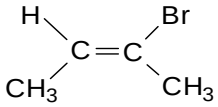


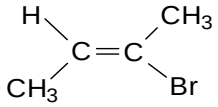
1-iodobutane	^{1}H Chemical Shift (δ) in ppm	1-butanol	^{1}H Chemical Shift (δ) in ppm
H1	2.70	**H1**	3.41
H2	1.40	**H2**	1.27
H3	1.08	**H3**	1.39
H4	0.64	**H4**	0.84
		-OH	1.95

Problem 303

(E)- and (Z)-2-butene

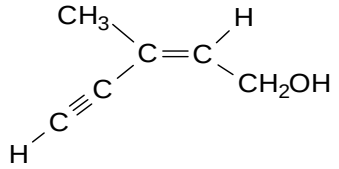




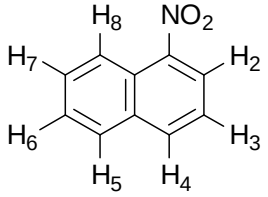


Problem 304

(*Z*)-3-methyl-2-penten-4-ynol

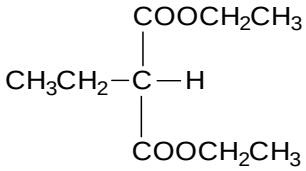


Problem 305

1-nitronaphthalene	
Proton	**Chemical Shift (δ) in ppm**
H2	8.22
H3	7.53
H4	8.10
H5	7.95
H6	7.62
H7	7.71
H8	**8.56**

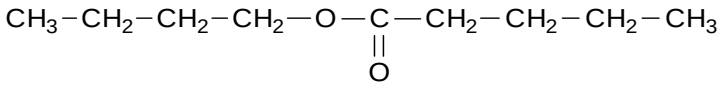
Problem 306

ethyl diethylmalonate



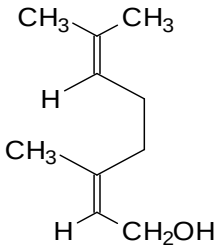
Problem 307

butyl valerate



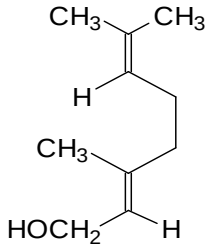
Problem 308

nerol



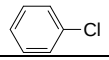
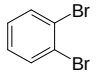
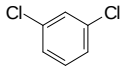
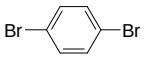
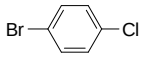
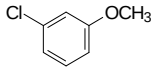
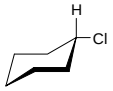
Problem 309

geraniol

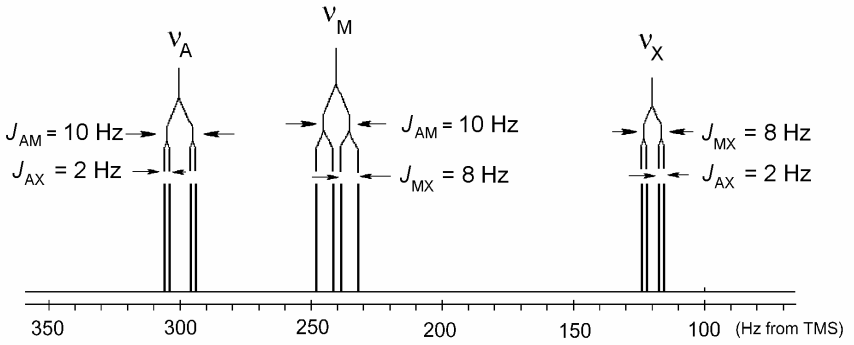


Chapter 9.4 – Analysis of NMR Spectra

Problem 310

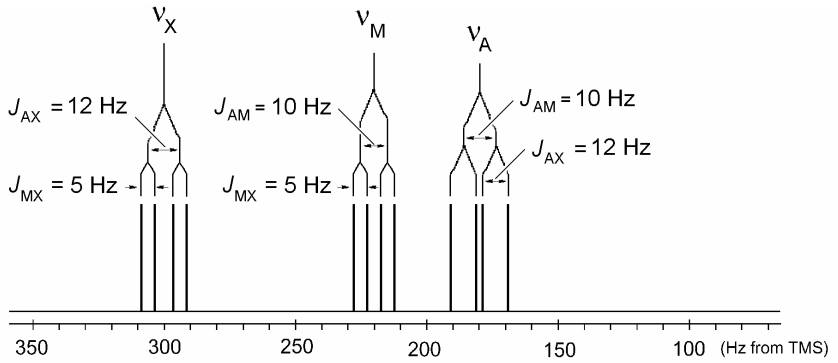
Structure		Number of 1H environments	Number of 13C environments
$CH_3-CO-CH_2CH_2CH_3$		4	5
$CH_3CH_2-CO-CH_2CH_3$		2	3
$CH_2=CHCH_2CH_3$		5	4
cis- $CH_3CH=CHCH_3$		2	2
trans-$CH_3CH=CHCH_3$		2	2
		1	1
		3	4
		2	3
		3	4
		1	2
		2	4
		5	7
	**slow chair-chair**	2	1
	**fast chair-chair**	1	1
	***rigid***	7	4

Problem 311



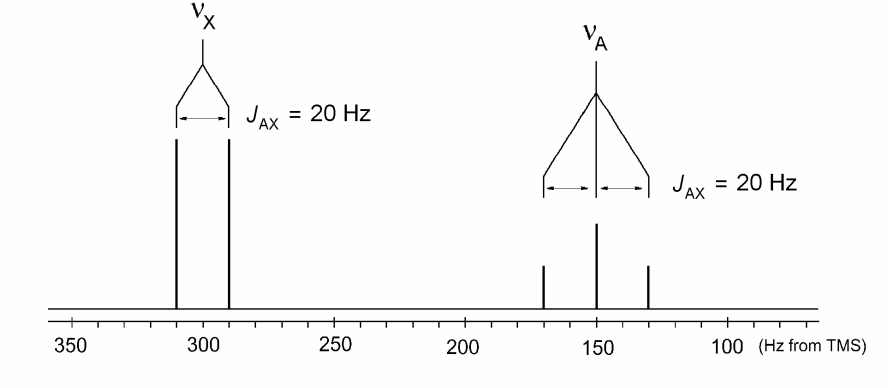
Chemical Shifts δ_A = 300 Hz / 60 MHz = 5.0 ppm
δ_M = 240 Hz / 60 MHz = 4.0 ppm
δ_X = 120 Hz / 60 MHz = 2.0 ppm

Problem 312



Chemical Shifts δ_A = 180 Hz / 200 MHz = 0.90 ppm
δ_M = 220 Hz / 200 MHz = 1.22 ppm
δ_X = 300 Hz / 200 MHz = 1.50 ppm

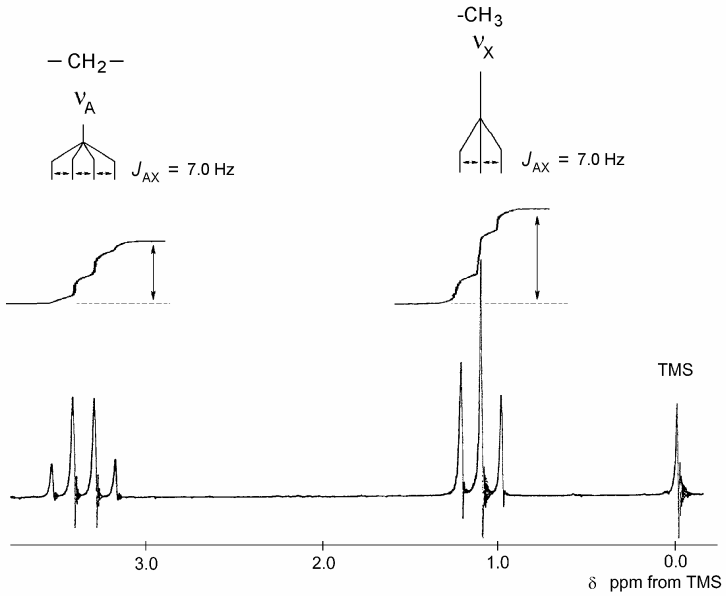
Problem 313



Chemical Shifts δ_A = 150 Hz / 400 MHz = 0.375 ppm
δ_X = 300 Hz / 400 MHz = 0.750 ppm

Problem 314

Spin System A_2X_3



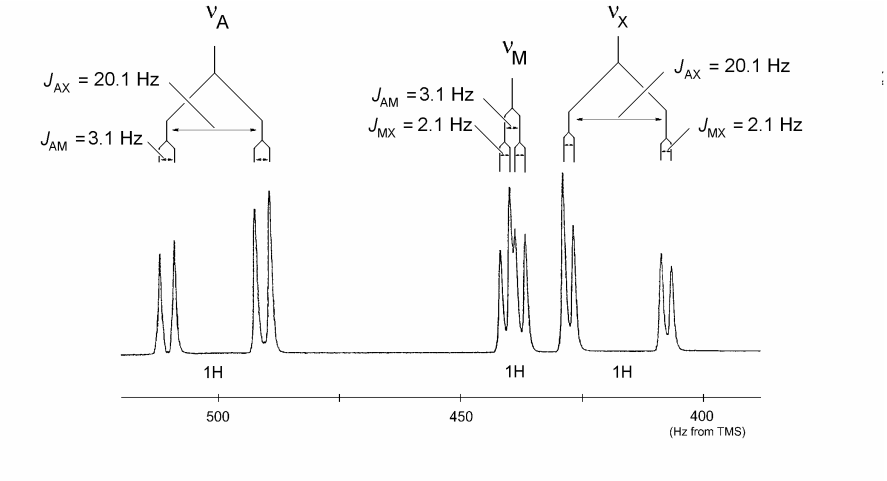
Chemical Shifts δ_A = 3.36 ppm = 3.36 x 60 = 202 Hz from TMS
δ_X = 1.11 ppm = 1.11 x 60 = 67 Hz from TMS

1st Order Analysis $\Delta\nu_{AX} = \nu_A - \nu_X$ = 202 - 67 = 135 Hz

$\Delta\nu_{AX} / J_{AX}$ = 135 / 7 = 19.3

This ratio is much greater than 3 so a 1st order analysis is justified.

Problem 315 **Spin System** AMX



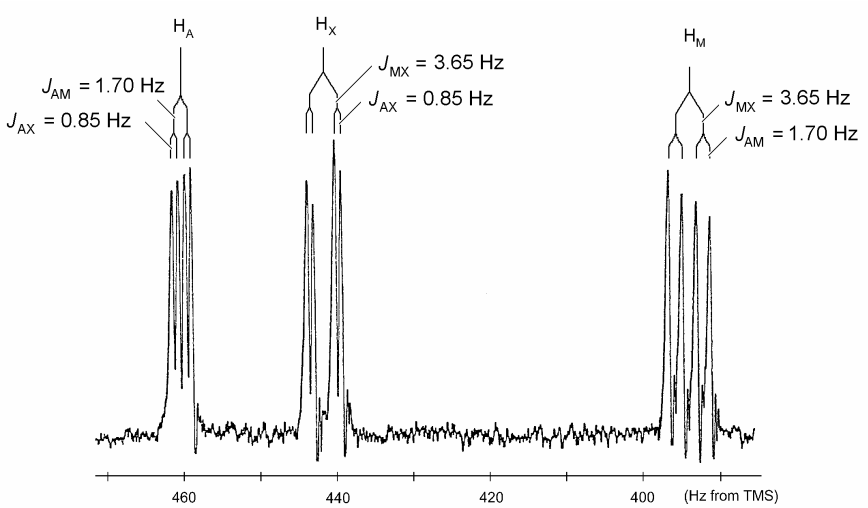
Chemical Shifts δ_A = 501 Hz / 100 MHz = 5.01 ppm
δ_M = 439 Hz / 100 MHz = 4.39 ppm
δ_X = 408 Hz / 100 MHz = 4.08 ppm

Coupling constants J_{AM} = 3.1 Hz
J_{AX} = 20.1 Hz
J_{MX} = 1.1 Hz

1st Order Analysis $\Delta\nu_{AM} = \nu_A - \nu_M$ = 501 - 439 = 62 Hz
$\Delta\nu_{A\Xi} = \nu_A - \nu_X$ = 501 - 408 = 93 Hz
$\Delta\nu_{M\Xi} = \nu_M - \nu_X$ = 439 - 408 = 31Hz
$\Delta\nu_{AM} / J_{AM}$ = 62 / 3.1 = 20.0
$\Delta\nu_{A\Xi} / J_{AX}$ = 93 / 20.1 = 4.6
$\Delta\nu_{M\Xi} / J_{MX}$ = 31 / 2.1 = 14.7

All ratios are greater than 3 so a 1st order analysis is justified.

Problem 316 **Spin System** AMX



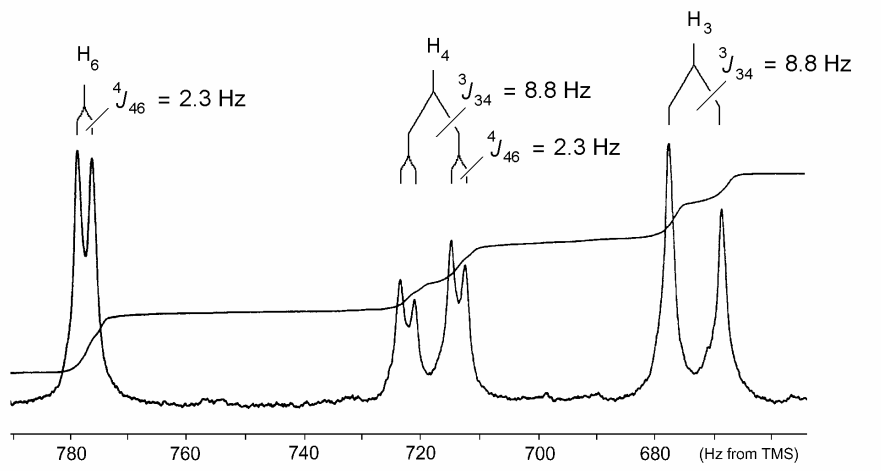
Chemical Shifts δ_A = 460 Hz / 60 MHz = 7.67 ppm
δ_X = 442 Hz / 60 MHz = 7.37 ppm
δ_M = 394 Hz / 60 MHz = 6.57ppm

Coupling constants J_{AM} = 1.70 Hz
J_{AX} = 0.85 Hz
J_{MX} = 3.65 Hz

1st Order Analysis $\Delta\nu_{AM} = \nu_A - \nu_M$ = 460 - 394 = 66 Hz
$\Delta\nu_{A\Xi} = \nu_A - \nu_X$ = 460 - 442 = 18 Hz
$\Delta\nu_{M\Xi} = \nu_M - \nu_X$ = 442 - 394 = 48 Hz
$\Delta\nu_{AM} / J_{AM}$ = 66 / 1.7 = 38.8
$\Delta\nu_{A\Xi} / J_{AX}$ = 18 / 0.85 = 21.2
$\Delta\nu_{M\Xi} / J_{MX}$ = 48 / 3.65 = 13.2

All ratios are greater than 3 so a 1st order analysis is justified.

Problem 317 **Spin System** AMX



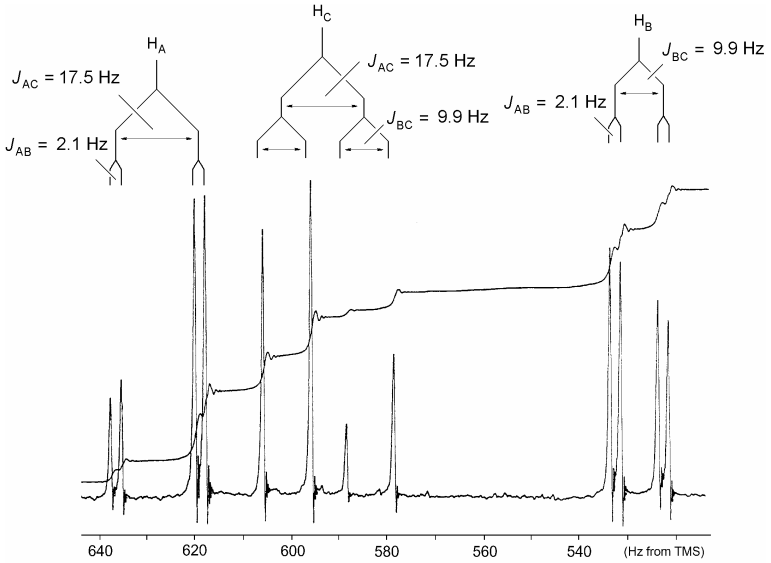
Chemical Shifts δ_3 = 673 Hz / 100 MHz = 6.73 ppm
δ_4 = 719 Hz / 100 MHz = 7.19 ppm
δ_6 = 777 Hz / 100 MHz = 7.77ppm

Coupling constants $^3J_{34}$ = 8.8 Hz
$^4J_{46}$ = 2.3 Hz
$^5J_{36}$ not resolved (< 1Hz)

1st Order Analysis $\Delta\nu_{34} = \nu_4 - \nu_3 = 719 - 673 = 46$ Hz
$\Delta\nu_{46} = \nu_6 - \nu_4 = 777 - 719 = 58$ Hz
$\Delta\nu_{36} = \nu_6 - \nu_3 = 777 - 673 = 104$ Hz
$\Delta\nu_{34} / J_{34} = 46 / 8.8 = 5.2$
$\Delta\nu_{46} / J_{46} = 58 / 2.3 = 25.2$
$\Delta\nu_{36} / J_{36} = 104 / <1 = >104$

All ratios are greater than 3 so a 1st order analysis is justified.

Problem 318 **Spin System** AMX



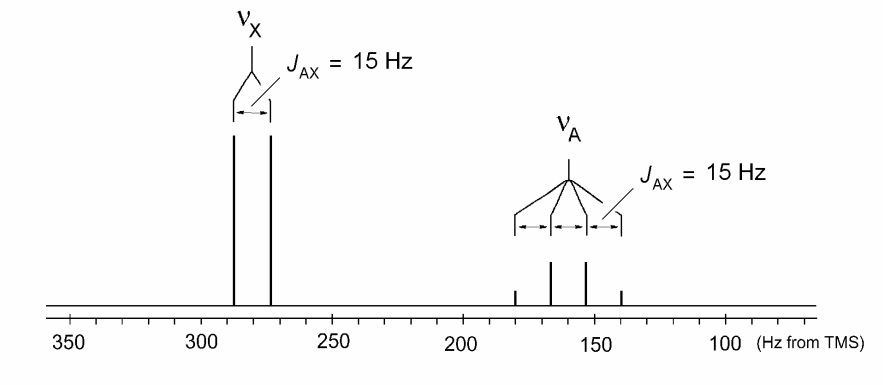
Chemical Shifts δ_A = 628 Hz / 100 MHz = 6.28 ppm
δ_B = 527 Hz / 100 MHz = 5.27 ppm
δ_C = 592 Hz / 100 MHz = 5.92 ppm

Coupling constants J_{AB} = 2.1 Hz; J_{AC} = 17.5 Hz; J_{BC} = 9.9 Hz

1st Order Analysis $\Delta\nu_{AB} = \nu_A - \nu_B = 628 - 527 = 101$ Hz
$\Delta\nu_{AC} = \nu_A - \nu_C = 628 - 592 = 36$ Hz
$\Delta\nu_{BC} = \nu_C - \nu_B = 592 - 527 = 65$ Hz
$\Delta\nu_{AB} / J_{AB} = 101 / 2.1 = 48.1$
$\Delta\nu_{AC} / J_{AC} = 36 / 17.5 = 2.1$
$\Delta\nu_{BC} / J_{BC} = 65 / 9.9 = 6.6$

2 out of 3 ratios are greater than 3 so this is borderline 1st order. The main deviation from 1st order is that intensities are severely distorted - a 1st order spectrum would have all lines of equal intensity. J_{AC} = 17.5 Hz indicates that H_A and H_C must be *trans*. J_{BC} = 9.9 Hz indicates H_A and H_C are *cis*.

Problem 319 **Spin System** AX_3



Chemical Shifts δ_A = 160 Hz / 60 MHz = 2.67 ppm
δ_X = 280 Hz / 60 MHz = 4.67 ppm

Problem 320 **Spin System** AX_3

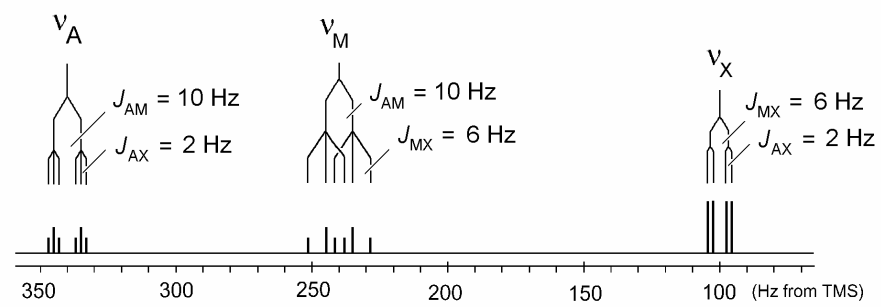
Chemical Shifts δ_A = 199 Hz / 100 MHz = 1.99 ppm
δ_X = 99 Hz / 100 MHz = 0.99 ppm

Coupling constants J_{AX} = 5 Hz

1st Order Analysis $\Delta\nu_{AX} = \nu_A - \nu_X$ = 199 - 99 = 100 Hz
$\Delta\nu_{AX} / J_{AX}$ = 100 / 5 = 20.0

$\Delta\nu_{AX} / J_{AX}$ is much greater than 3 so a 1st order analysis is justified.

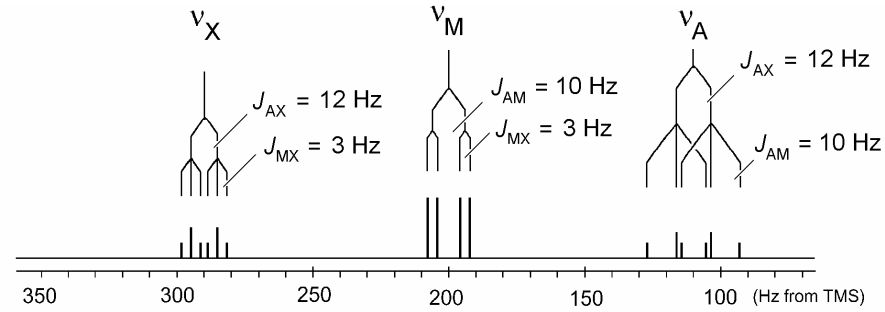
Problem 321 **4 Spin System** AMX_2



Chemical Shifts

δ_A = 340 Hz / 60 MHz = 5.67 ppm
δ_M = 240 Hz / 60 MHz = 4.00 ppm
δ_X = 100 Hz / 60 MHz = 1.67 ppm

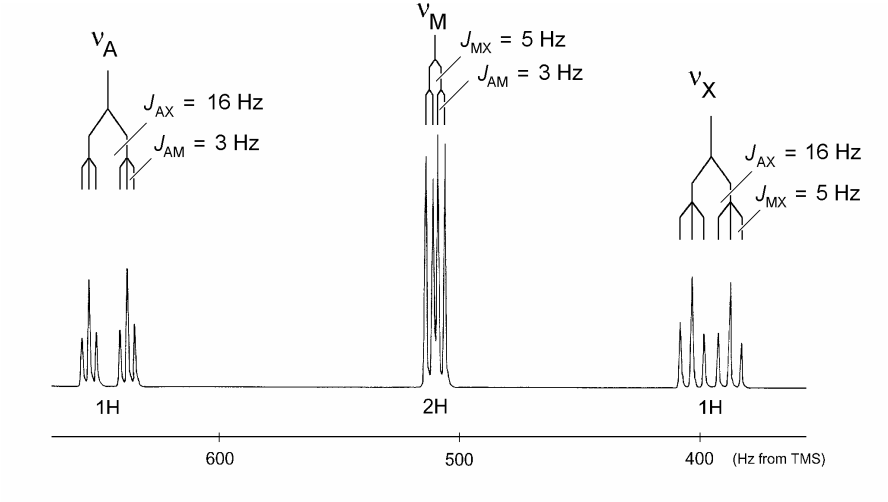
Problem 322 **4 Spin System** AM_2X



Chemical Shifts

δ_A = 110 Hz / 60 MHz = 1.83ppm
δ_M = 200 Hz / 60 MHz = 3.33 ppm
δ_X = 290 Hz / 60 MHz = 4.83 ppm

Problem 323 4 Spin System AM_2X



Chemical Shifts δ_A = 646 Hz / 100 MHz = 6.46 ppm
δ_M = 510 Hz / 100 MHz = 5.10 ppm
δ_X = 395 Hz / 100 MHz = 3.95 ppm

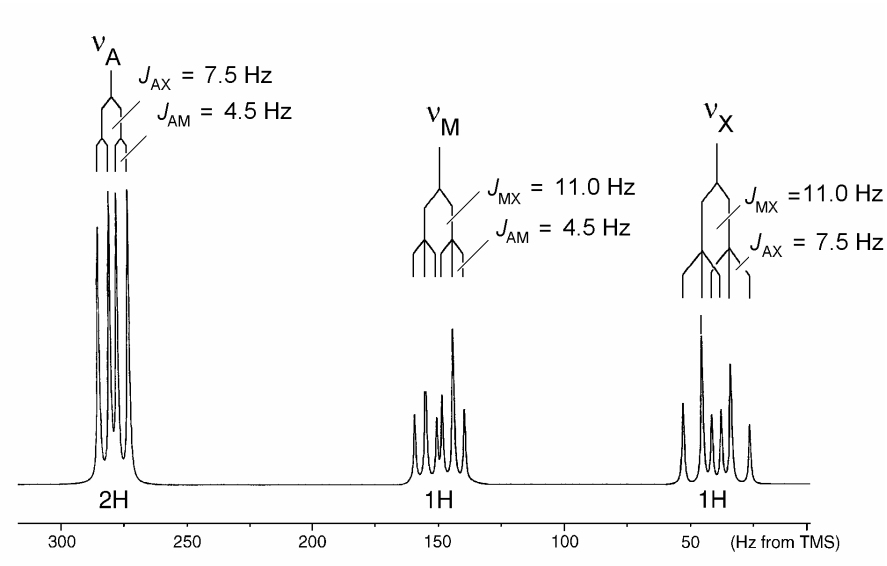
Coupling constants J_{AM} = 3 Hz; J_{AX} = 16 Hz; J_{MX} = 5 Hz;

1st Order Analysis $\Delta\nu_{AX} = \nu_A - \nu_X$ = 646 - 395 = 251 Hz
$\Delta\nu_{AM} = \nu_A - \nu_M$ = 646 - 510 = 136 Hz
$\Delta\nu_{MX} = \nu_M - \nu_X$ = 510 - 395 = 115 Hz

$\Delta\nu_{AX} / J_{AX}$ = 251 / 16 = 15.7
$\Delta\nu_{AM} / J_{AM}$ = 136 / 3 = 45.3
$\Delta\nu_{MX} / J_{MX}$ = 115 / 5 = 23.0

All ratios are significantly greater than 3 so a 1st order analysis is justified.

Problem 324 4 Spin System A_2MX



Chemical Shifts δ_A = 279 Hz / 100 MHz = 2.79 ppm
δ_M = 149 Hz / 100 MHz = 1.49 ppm
δ_X = 39 Hz / 100 MHz = 0.39 ppm

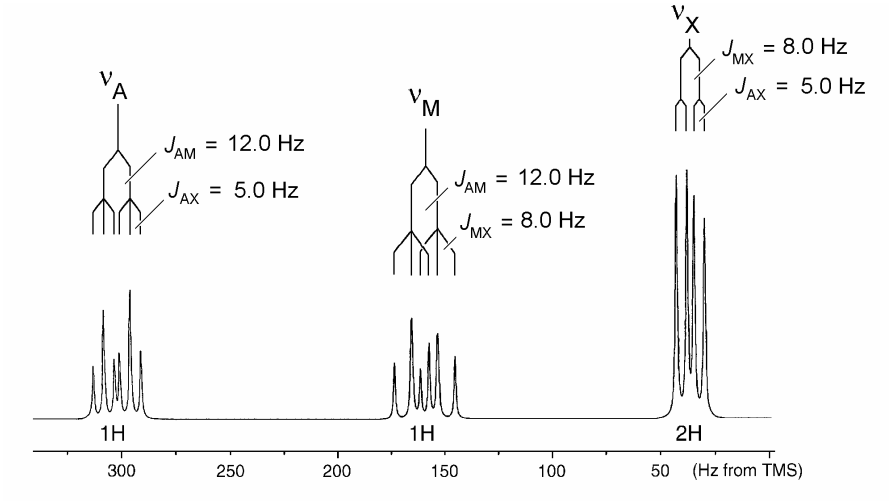
Coupling constants J_{AM} = 4.5 Hz; J_{AX} = 7.5 Hz; J_{MX} = 11.0 Hz;

1st Order Analysis $\Delta\nu_{AX} = \nu_A - \nu_X$ = 279 - 39 = 240 Hz
$\Delta\nu_{AM} = \nu_A - \nu_M$ = 279 - 149 = 130 Hz
$\Delta\nu_{MX} = \nu_M - \nu_X$ = 149 - 39 = 110 Hz

$\Delta\nu_{AX} / J_{AX}$ = 240 / 7.5 = 32.0
$\Delta\nu_{AM} / J_{AM}$ = 130 / 4.5 = 28.9
$\Delta\nu_{MX} / J_{MX}$ = 110 / 11 = 10.0

All ratios are significantly greater than 3 so a 1st order analysis is justified.

Problem 325 4 Spin System AMX_2



Chemical Shifts δ_A = 302 Hz / 100 MHz = 3.02 ppm
δ_M = 160 Hz / 100 MHz = 1.60 ppm
δ_X = 37 Hz / 100 MHz = 0.37 ppm

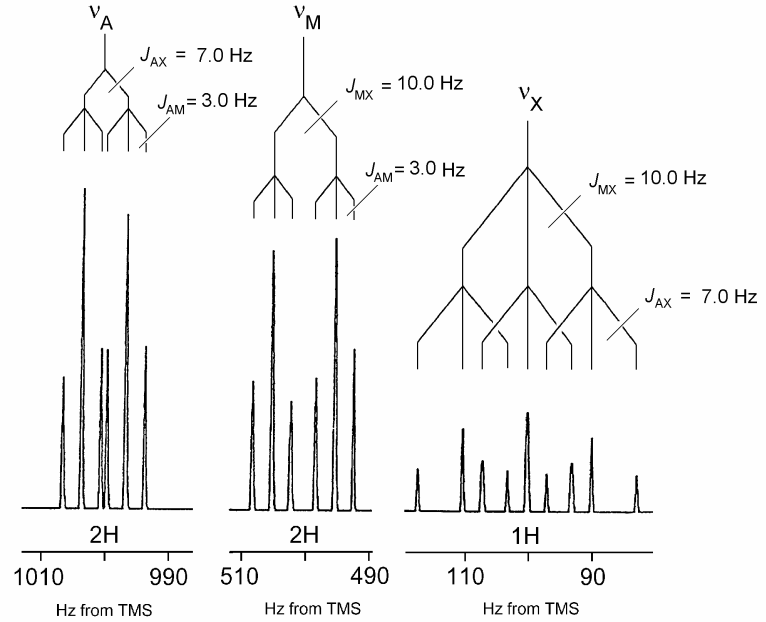
Coupling constants J_{AM} = 12.0 Hz; J_{AX} = 5.0 Hz; J_{MX} = 8.0 Hz;

1st Order Analysis $\Delta\nu_{AX} = \nu_A - \nu_X$ = 302 - 37 = 265 Hz
$\Delta\nu_{AM} = \nu_A - \nu_M$ = 302 - 160 = 142 Hz
$\Delta\nu_{MX} = \nu_M - \nu_X$ = 160 - 37 = 123 Hz

$\Delta\nu_{AX} / J_{AX}$ = 265 / 5.0 = 53.0
$\Delta\nu_{AM} / J_{AM}$ = 142 / 12.0 = 11.8
$\Delta\nu_{MX} / J_{MX}$ = 123 / 8.0 = 15.4

All ratios are significantly greater than 3 so a 1st order analysis is justified.

Problem 326 5 Spin System A_2M_2X



Chemical Shifts δ_A = 1000 Hz / 200 MHz = 5.0 ppm
δ_M = 500 Hz / 200 MHz = 2.5 ppm
δ_X = 100 Hz / 200 MHz = 0.5 ppm

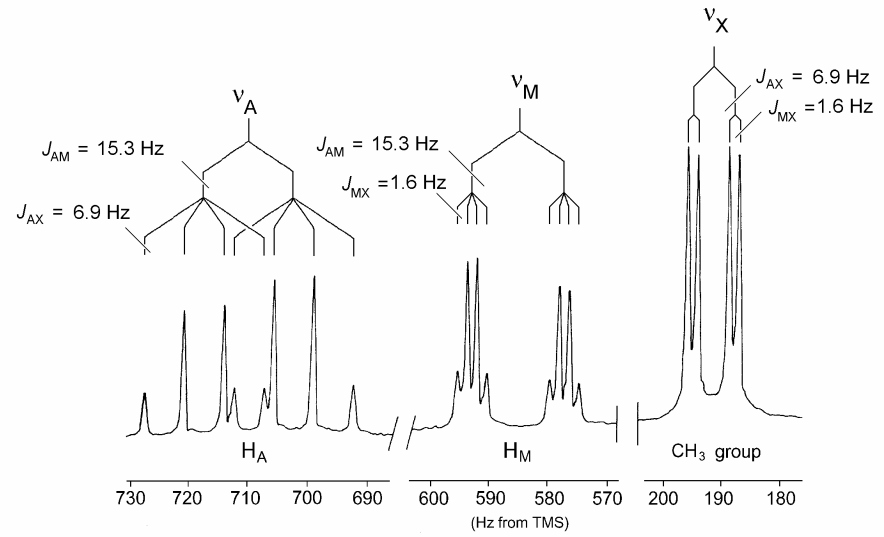
Coupling constants J_{AM} = 3.0 Hz; J_{AX} = 7.0 Hz; J_{MX} = 10.0 Hz;

1st Order Analysis $\Delta\nu_{AX} = \nu_A - \nu_X$ = 1000 - 100 = 900 Hz
$\Delta\nu_{AM} = \nu_A - \nu_M$ = 1000 - 500 = 500 Hz
$\Delta\nu_{MX} = \nu_M - \nu_X$ = 500 - 100 = 400 Hz

$\Delta\nu_{AX} / J_{AX}$ = 900 / 7.0 = 128.6
$\Delta\nu_{AM} / J_{AM}$ = 500 / 3.0 = 166.7
$\Delta\nu_{MX} / J_{MX}$ = 400 / 10.0 = 40.0

All ratios are significantly greater than 3 so a 1st order analysis is justified.

Problem 327 5 Spin System AMX_3



Chemical Shifts δ_A = 710 Hz / 100 MHz = 7.10 ppm
δ_M = 585 Hz / 100 MHz = 5.85 ppm
δ_X = 192 Hz / 100 MHz = 1.92 ppm

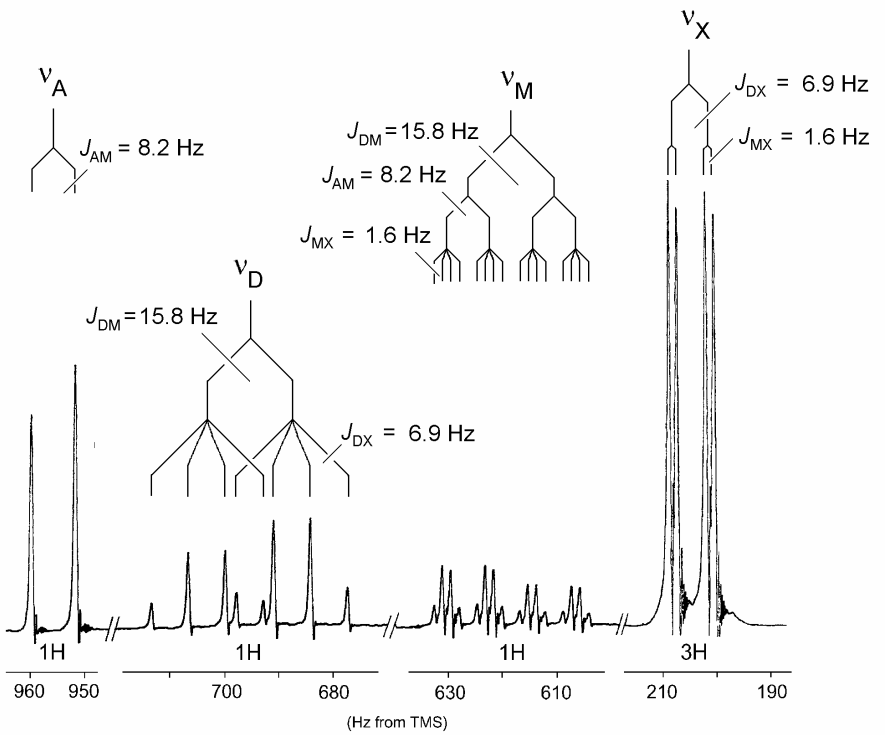
Coupling constants J_{AM} = 15.3 Hz; J_{AX} = 6.9 Hz; J_{MX} = 1.6 Hz;

1st Order Analysis $\Delta\nu_{AX} = \nu_A - \nu_X$ = 710 - 192 = 518 Hz
$\Delta\nu_{AM} = \nu_A - \nu_M$ = 710 - 585 = 125 Hz
$\Delta\nu_{MX} = \nu_M - \nu_X$ = 585 - 192 = 393 Hz

$\Delta\nu_{AX} / J_{AX}$ = 518 / 6.9 = 84.7
$\Delta\nu_{AM} / J_{AM}$ = 125 / 15.3 = 8.2
$\Delta\nu_{MX} / J_{MX}$ = 393 / 1.6 = 245.6

All ratios are significantly greater than 3 so a 1st order analysis is justified. J_{AM} = 15.3 Hz is typical of a coupling between vinylic protons which are *trans* to each other (see Section 5.7)

Problem 328 5 Spin System $ADMX_3$



Chemical Shifts

δ_A = 956 Hz / 100 MHz = 9.56 ppm;
δ_D = 695 Hz / 100 MHz = 6.95 ppm;
δ_M = 619 Hz / 100 MHz = 6.19 ppm;
δ_X = 205 Hz / 100 MHz = 2.05 ppm;

Coupling constants

J_{AD}= < 1 Hz; J_{AM} = 8.2 Hz; J_{AX} = < 1 Hz;
J_{DM} = 15.8 Hz; J_{DX} = 6.9 Hz; J_{MX} = 1.6Hz;

1st Order Analysis

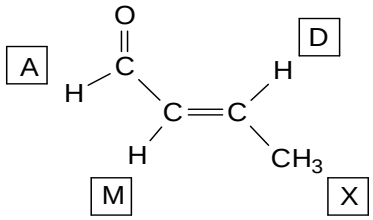
$\Delta\nu_{AD} = \nu_A - \nu_D = 956 - 695 = 261$ Hz
$\Delta\nu_{AM} = \nu_A - \nu_M = 956 - 619 = 337$ Hz
$\Delta\nu_{AX} = \nu_A - \nu_X = 956 - 205 = 751$ Hz
$\Delta\nu_{DM} = \nu_D - \nu_M = 695 - 619 = 76$ Hz
$\Delta\nu_{DX} = \nu_D - \nu_X = 695 - 205 = 490$ Hz
$\Delta\nu_{MX} = \nu_M - \nu_X = 619 - 205 = 414$ Hz

$\Delta\nu_{AD} / J_{AD} = 261 / <1 = >261$
$\Delta\nu_{AM} / J_{AM} = 337 / 8.2 = 41.1$
$\Delta\nu_{AX} / J_{AX} = 751 / <1 = >751$
$\Delta\nu_{DM} / J_{DM} = 76 / 15.8 = 4.8$
$\Delta\nu_{DX} / J_{DX} = 490 / 6.9 = 71.0$
$\Delta\nu_{MX} / J_{MX} = 414 / 1.6 = 258.8$

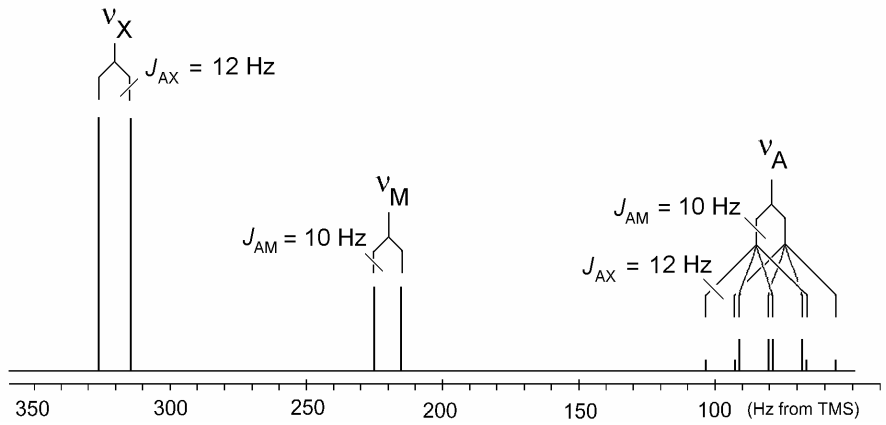
All ratios are significantly greater than 3 so a 1st order analysis is justified.

The critical coupling constant is J_{DM} = 15.8 Hz which is typical of a coupling between vinylic protons which are *trans* to each other (see Section 5.7).

The compound is:



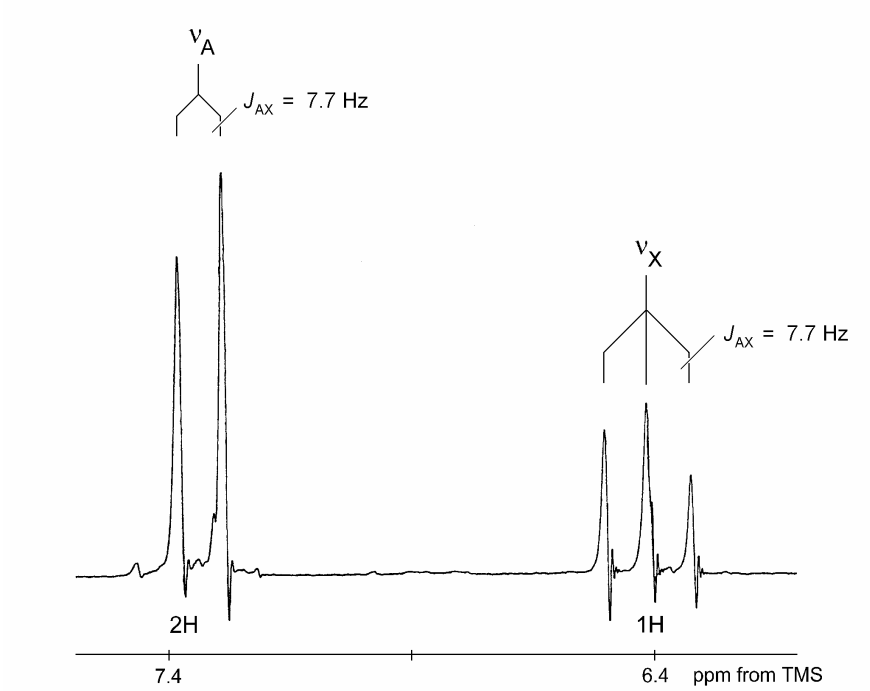
Problem 329 **5 Spin System** AMX_3



Chemical Shifts

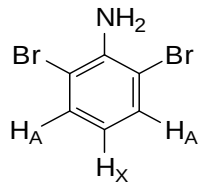
δ_A = 80 Hz / 60 MHz = 1.33 ppm
δ_M = 220 Hz / 60 MHz = 3.67 ppm
δ_X = 320 Hz / 60 MHz = 5.33 ppm

Problem 330 **3 Spin System** A_2X



Of the 6 isomeric anilines, only compounds **4** and **6** have the correct symmetry to give a spectrum with only two chemical shifts in the aromatic region, in the ratio 2:1.

Both **4** and **6** would give A_2X spin systems. The measured coupling constant is 7.7 Hz which is in the range for protons which are *ortho* to each other. Compound **4** is the correct answer.



Problem 331

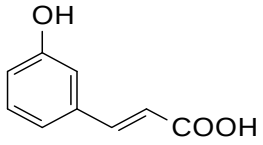
The spectrum is obtained after D_2O exchange so the carboxylic acid and phenolic protons will not be present and the spectrum only contains the aromatic and vinylic protons.

The spectrum shows 6 distinct resonances therefore compounds **5** and **6** can be eliminated because they would each have only 4 resonances (on symmetry grounds).

The proton at about δ 7.1 shows no large coupling (> 7 Hz), this means that it has no protons *ortho* to it. This eliminates compounds **1** and **2** since all protons in these compounds will have at least one large *ortho* coupling.

Compounds **3** and **4** differ by the stereochemistry at the double bond. The proton at δ 6.4 is clearly one of the vinylic protons and it is coupled to the other vinylic proton at δ 7.6. The coupling constant is 16 Hz and this characteristic of vinylic protons which are *trans* to each other.

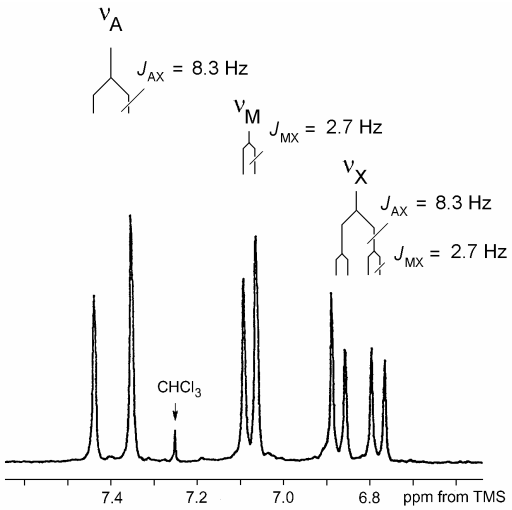
The correct answer is compound **3**.

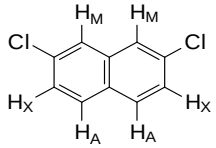


Problem 332

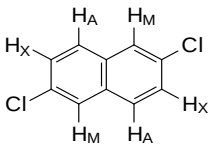
All of the protons in the ^1H spectrum 1,5-dichoronaphthalene have protons which are *ortho* to them. This means that every proton must have at least one large (>7 Hz) *ortho* coupling. The spectrum has one proton (at δ 7.1) which has only a small coupling so this cannot be the spectrum of 1,5-dichloronaphthalene.

The spectrum is an AMX spectrum with couplings between A and X of about 8.3 Hz (typical of an *ortho* coupling) and coupling between M and X of about 2.7 Hz (typical of a *meta* coupling). Two possible structure are given below.





2,7-dichloronaphthalene



2,6-dichloronaphthalene