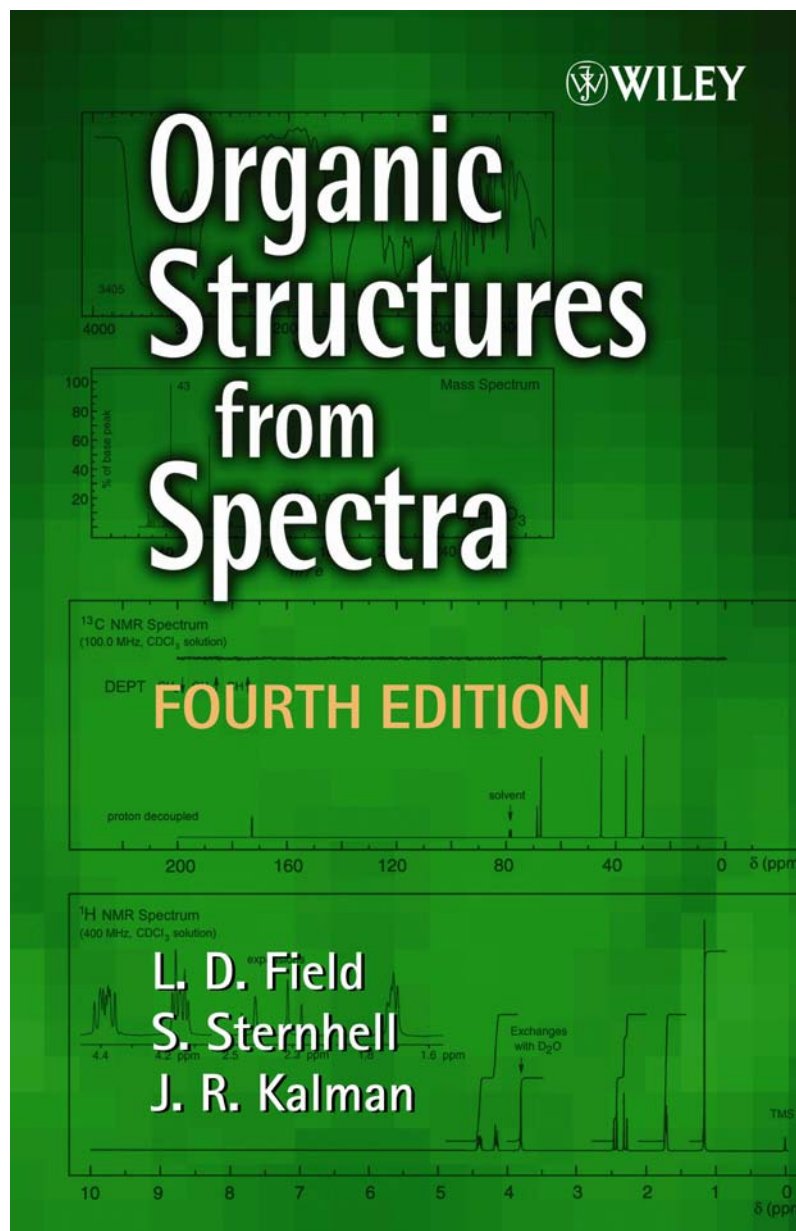



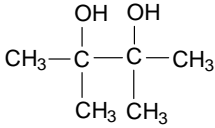
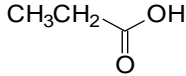
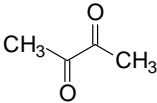
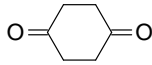
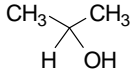
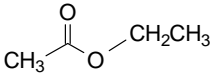
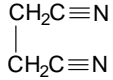

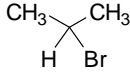
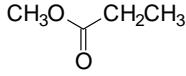
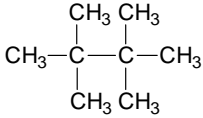
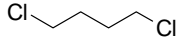
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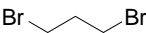
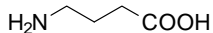
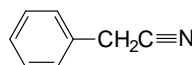
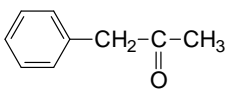
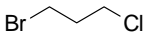
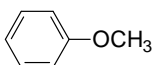
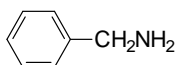
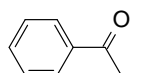
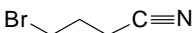
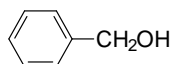
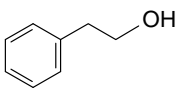
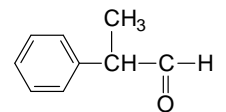
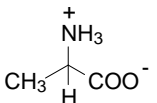
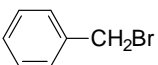
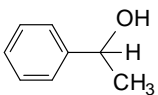
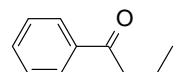
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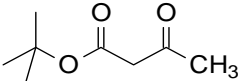
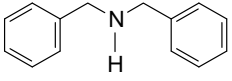
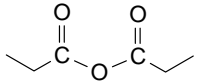
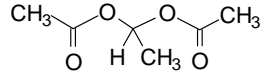
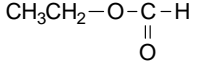
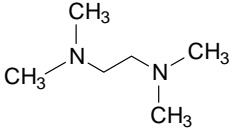
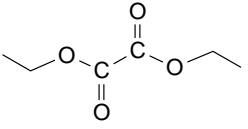
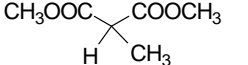
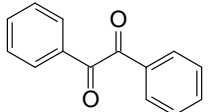
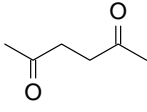
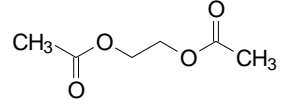
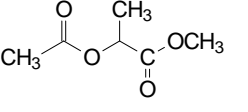
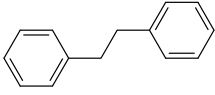
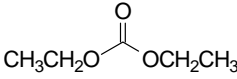
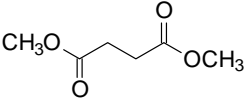
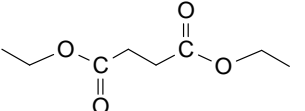
<p><b>1</b></p>  <p>2-butanone <math>C_4H_8O</math></p>	<p><b>5</b></p> <p><math>BrCH_2-CH_2Br</math></p> <p>1,2-dibromoethane <math>C_2H_4Br_2</math></p>	<p><b>9</b></p>  <p>pinacol <math>C_6H_{14}O_2</math></p>	<p><b>13</b></p> <p><math>Cl_2CH-CH_3</math></p> <p>1,1-dichloroethane <math>C_2H_4Cl_2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

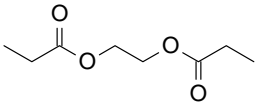
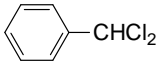
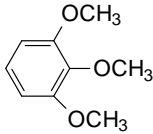
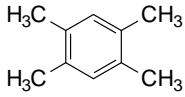
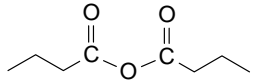
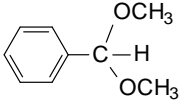
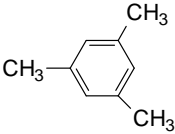
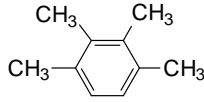
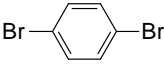
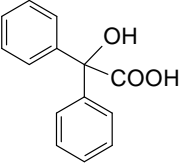
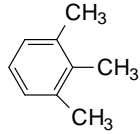
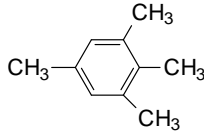
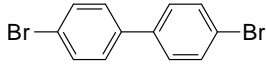
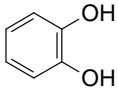
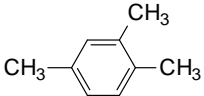
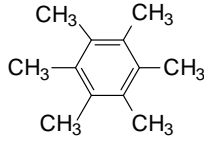
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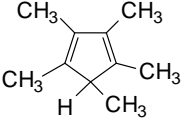
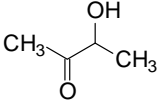
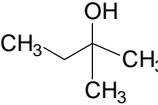
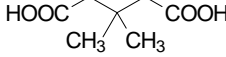
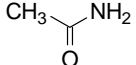
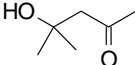
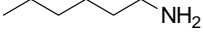
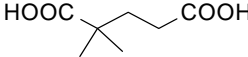
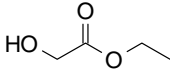
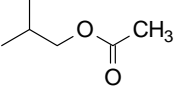
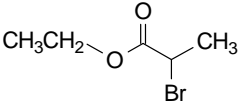
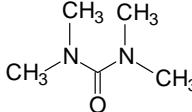
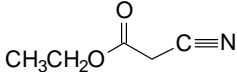
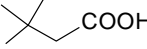
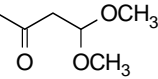

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<p><b>17</b></p>  <p>1,3-dibromopropane</p> <p><math>C_3H_6Br_2</math></p>	<p><b>21</b></p>  <p>4-aminobutyric acid</p> <p><math>C_4H_9NO_2</math></p>	<p><b>25</b></p>  <p>benzyl cyanide</p> <p><math>C_8H_7N</math></p>	<p><b>29</b></p>  <p>benzyl methyl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

<p>33</p>  <p><i>t</i>-butyl acetoacetate <math>C_8H_{14}O_3</math></p>	<p>37</p>  <p>dibenzylamine <math>C_{14}H_{15}N</math></p>	<p>41</p>  <p>propionic anhydride <math>C_6H_{10}O_3</math></p>	<p>45</p>  <p>1,1-diacetoxyethane <math>C_6H_{10}O_4</math></p>
<p>34</p>  <p>ethyl formate <math>C_3H_6O_2</math></p>	<p>38</p>  <p><i>N,N,N,N</i>-tetramethyl-1,2-ethanediamine <math>C_6H_{16}N_2</math></p>	<p>42</p>  <p>diethyl oxalate <math>C_6H_{10}O_4</math></p>	<p>46</p>  <p>dimethyl methylmalonate <math>C_6H_{10}O_4</math></p>
<p>35</p>  <p>benzil <math>C_{14}H_{10}O_2</math></p>	<p>39</p>  <p>2,5-hexanedione <math>C_6H_{10}O_2</math></p>	<p>43</p>  <p>ethylene glycol diacetate <math>C_6H_{10}O_4</math></p>	<p>47</p>  <p>methyl acetylacrylate <math>C_6H_{10}O_4</math></p>
<p>36</p>  <p>1,2-diphenylethane <math>C_{14}H_{14}</math></p>	<p>40</p>  <p>diethyl carbonate <math>C_5H_{10}O_3</math></p>	<p>44</p>  <p>dimethyl succinate <math>C_6H_{10}O_4</math></p>	<p>48</p>  <p>diethyl succinate <math>C_8H_{14}O_4</math></p>


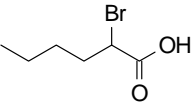
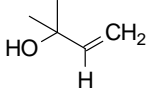
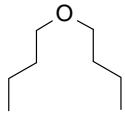
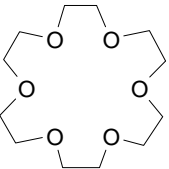
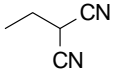
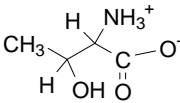
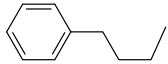
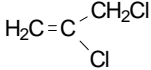
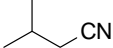
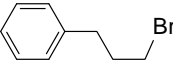
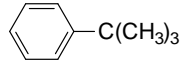
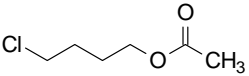
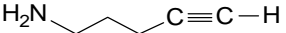
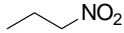
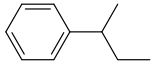
<p>49</p>  <p>ethylene glycol dipropionate</p> <p><math>C_8H_{14}O_4</math></p>	<p>53</p>  <p><math>\alpha,\alpha</math>-dichlorotoluene</p> <p><math>C_7H_6Cl_2</math></p>	<p>57</p>  <p>1,2,3-trimethoxybenzene</p> <p><math>C_9H_{12}O_3</math></p>	<p>61</p>  <p>durene</p> <p><math>C_{10}H_{14}</math></p>
<p>50</p>  <p>butyric anhydride</p> <p><math>C_8H_{14}O_3</math></p>	<p>54</p>  <p>benzaldehyde dimethylacetal</p> <p><math>C_9H_{12}O_2</math></p>	<p>58</p>  <p>mesitylene</p> <p><math>C_9H_{12}</math></p>	<p>62</p>  <p>1,2,3,4-tetramethylbenzene</p> <p><math>C_{10}H_{14}</math></p>
<p>51</p>  <p>1,4-dibromobenzene</p> <p><math>C_6H_4Br_2</math></p>	<p>55</p>  <p>benzilic acid</p> <p><math>C_{14}H_{12}O_3</math></p>	<p>59</p>  <p>1,2,3-trimethylbenzene</p> <p><math>C_9H_{12}</math></p>	<p>63</p>  <p>1,2,3,5-tetramethylbenzene</p> <p><math>C_{10}H_{14}</math></p>
<p>52</p>  <p>4,4'-dibromobiphenyl</p> <p><math>C_{12}H_8Br_2</math></p>	<p>56</p>  <p>catechol</p> <p><math>C_6H_6O_2</math></p>	<p>60</p>  <p>1,2,4-trimethylbenzene</p> <p><math>C_9H_{12}</math></p>	<p>64</p>  <p>hexamethylbenzene</p> <p><math>C_{12}H_{18}</math></p>

<p><b>65</b></p>  <p>1,2,3,4,5,- pentamethylcyclopentadiene <math>C_{10}H_{16}</math></p>	<p><b>69</b></p>  <p>3-hydroxybutanone (acetoin) <math>C_4H_8O_2</math></p>	<p><b>73</b></p>  <p>2-methyl-2-butanol (<i>t</i>-amyl alcohol) <math>C_5H_{12}O</math></p>	<p><b>77</b></p>  <p>3,3-dimethylglutaric acid <math>C_7H_{12}O_4</math></p>
<p><b>66</b></p>  <p>acetamide <math>C_2H_5NO</math></p>	<p><b>70</b></p>  <p>4-hydroxy-4-methyl-2- pentanone <math>C_6H_{12}O_2</math></p>	<p><b>74</b></p>  <p>hexylamine <math>C_6H_{15}N</math></p>	<p><b>78</b></p>  <p>2,2-dimethylpentanedioic acid <math>C_7H_{12}O_4</math></p>
<p><b>67</b></p>  <p>ethyl glycolate <math>C_4H_8O_3</math></p>	<p><b>71</b></p>  <p>isobutyl acetate <math>C_6H_{12}O_2</math></p>	<p><b>75</b></p>  <p>ethyl 2-bromopropionate <math>C_5H_9O_2Br</math></p>	<p><b>79</b></p>  <p>tetramethylurea <math>C_5H_{12}N_2O</math></p>
<p><b>68</b></p>  <p>ethyl cyanoacetate <math>C_5H_7NO_2</math></p>	<p><b>72</b></p>  <p>3,3-dimethylbutyric acid <math>C_6H_{12}O_2</math></p>	<p><b>76</b></p>  <p>4,4-dimethoxy-2-butanone <math>C_6H_{12}O_3</math></p>	<p><b>80</b></p>  <p>1,3-dioxan <math>C_4H_8O_2</math></p>

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ORGANIC STRUCTURES FROM SPECTRA – 4th EDITION  
L D Field, S Sternhell and J R Kalman

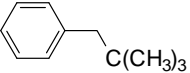
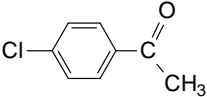
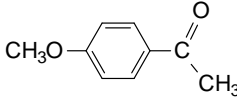
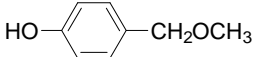
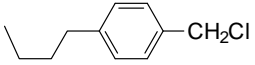
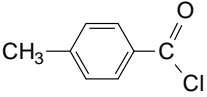
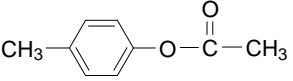
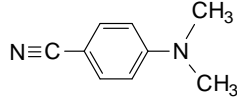
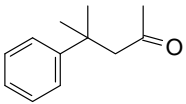
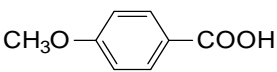
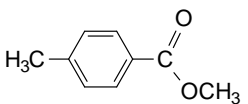
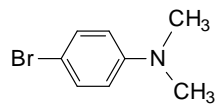
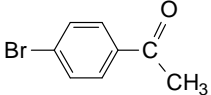
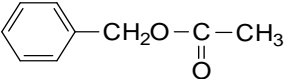
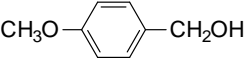
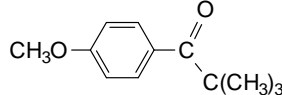
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<p>81</p>  <p>1,4-dioxan</p> <p><math>C_4H_8O_2</math></p>	<p>85</p>  <p>2-bromohexanoic acid</p> <p><math>C_6H_{11}O_2Br</math></p>	<p>89</p>  <p>2-methylbut-3-en-2-ol</p> <p><math>C_5H_{10}O</math></p>	<p>93</p>  <p>dibutyl ether</p> <p><math>C_8H_{18}O</math></p>
<p>82</p>  <p>18-crown-6</p> <p><math>C_{12}H_{24}O_6</math></p>	<p>86</p>  <p>2-ethylmalononitrile</p> <p><math>C_5H_6N_2</math></p>	<p>90</p>  <p>threonine</p> <p><math>C_4H_9NO_3</math></p>	<p>94</p>  <p>butylbenzene</p> <p><math>C_{10}H_{14}</math></p>
<p>83</p>  <p>2,3-dichloropropene</p> <p><math>C_3H_4Cl_2</math></p>	<p>87</p>  <p>3-methylbutyronitrile</p> <p><math>C_5H_9N</math></p>	<p>91</p>  <p>1-bromo-3-phenylpropane</p> <p><math>C_9H_{11}Br</math></p>	<p>95</p>  <p><i>t</i>-butylbenzene</p> <p><math>C_{10}H_{14}</math></p>
<p>84</p>  <p>4-chlorobutyl acetate</p> <p><math>C_6H_{11}O_2Cl</math></p>	<p>88</p>  <p>5-amino-1-pentyne</p> <p><math>C_5H_9N</math></p>	<p>92</p>  <p>1-nitropropane</p> <p><math>C_3H_7NO_2</math></p>	<p>96</p>  <p><i>sec</i>-butylbenzene</p> <p><math>C_{10}H_{14}</math></p>

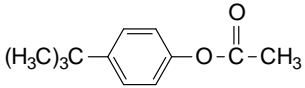
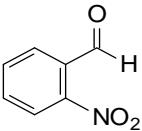
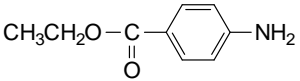
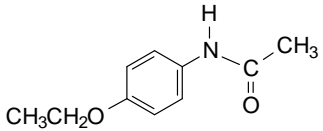
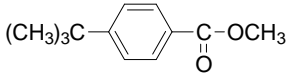
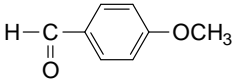
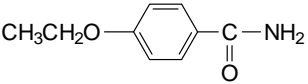
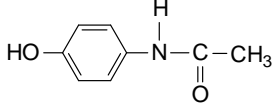
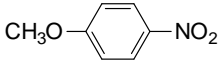
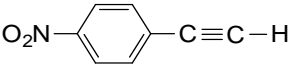
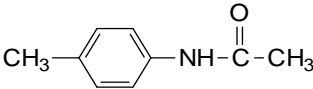
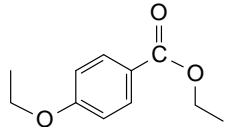
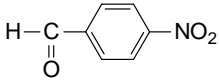
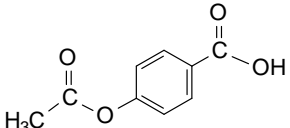
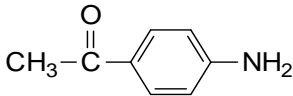
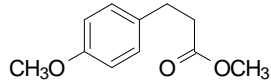
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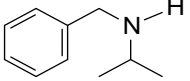
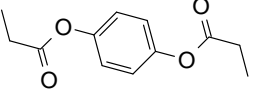
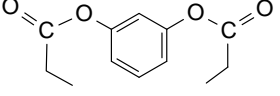
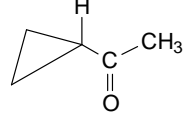
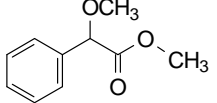
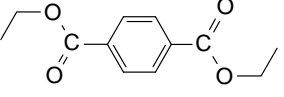
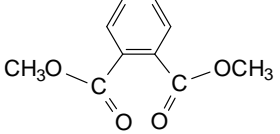
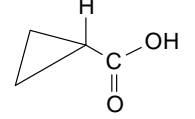
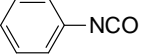
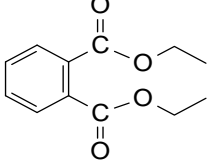
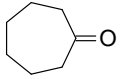
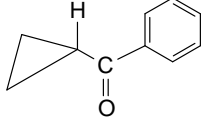
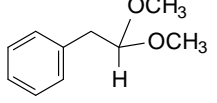
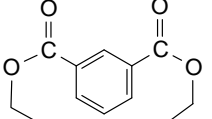
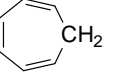
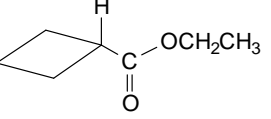
ORGANIC STRUCTURES FROM SPECTRA – 4th EDITION  
L D Field, S Sternhell and J R Kalman

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<p>97</p>  <p>neopentylbenzene <math>C_{11}H_{16}</math></p>	<p>101</p>  <p><i>p</i>-chloroacetophenone <math>C_8H_7OCl</math></p>	<p>105</p>  <p>4-methoxyacetophenone <math>C_9H_{10}O_2</math></p>	<p>109</p>  <p>4-methoxymethylphenol <math>C_8H_{10}O_2</math></p>
<p>98</p>  <p>4-(<i>n</i>-butyl)-<math>\alpha</math>-chlorotoluene <math>C_{11}H_{15}Cl</math></p>	<p>102</p>  <p><i>p</i>-toluy chloride <math>C_8H_7OCl</math></p>	<p>106</p>  <p><i>p</i>-cresyl acetate <math>C_9H_{10}O_2</math></p>	<p>110</p>  <p>4-dimethylaminobenzonitrile <math>C_9H_{10}N_2</math></p>
<p>99</p>  <p>4-methyl-4-phenyl-2-pentanone <math>C_{12}H_{16}O</math></p>	<p>103</p>  <p><i>p</i>-anisic acid <math>C_8H_8O_3</math></p>	<p>107</p>  <p>methyl <i>p</i>-toluate <math>C_9H_{10}O_2</math></p>	<p>111</p>  <p><i>p</i>-bromo-<i>N,N</i>-dimethylaniline <math>C_8H_{10}NBr</math></p>
<p>100</p>  <p><i>p</i>-bromoacetophenone <math>C_8H_7OBr</math></p>	<p>104</p>  <p>benzyl acetate <math>C_9H_{10}O_2</math></p>	<p>108</p>  <p><i>p</i>-methoxybenzyl alcohol <math>C_8H_{10}O_2</math></p>	<p>112</p>  <p><i>p</i>-anisyl <i>t</i>-butyl ketone <math>C_{12}H_{16}O_2</math></p>



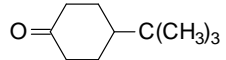
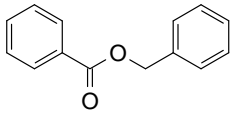
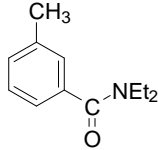
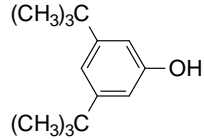
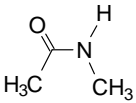
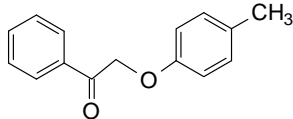
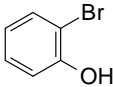
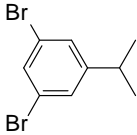
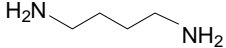
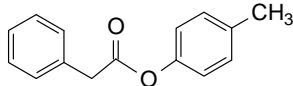
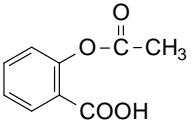
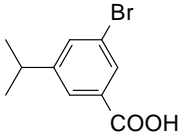
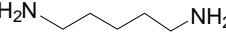
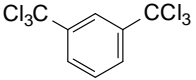
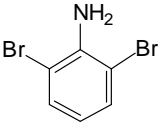
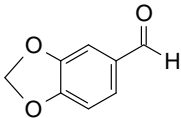
<p><b>113</b></p>  <p>4-<i>t</i>-butylphenyl acetate <math>C_{12}H_{16}O_2</math></p>	<p><b>117</b></p>  <p><i>o</i>-nitrobenzaldehyde <math>C_7H_5NO_3</math></p>	<p><b>121</b></p>  <p>ethyl <i>p</i>-aminobenzoate <math>C_9H_{11}NO_2</math></p>	<p><b>125</b></p>  <p><i>p</i>-ethoxyacetanilide (phenacetin) <math>C_{10}H_{13}NO_2</math></p>
<p><b>114</b></p>  <p>methyl 4-<i>t</i>-butylbenzoate <math>C_{12}H_{16}O_2</math></p>	<p><b>118</b></p>  <p>4-methoxybenzaldehyde <math>C_8H_8O_2</math></p>	<p><b>122</b></p>  <p><i>p</i>-ethoxybenzamide <math>C_9H_{11}NO_2</math></p>	<p><b>126</b></p>  <p><i>p</i>-hydroxyacetanilide (paracetamol) <math>C_8H_9NO_2</math></p>
<p><b>115</b></p>  <p><i>p</i>-nitroanisole <math>C_7H_7NO_3</math></p>	<p><b>119</b></p>  <p>4-nitrophenylacetylene <math>C_8H_5NO_2</math></p>	<p><b>123</b></p>  <p>4-methylacetanilide <math>C_8H_9NO</math></p>	<p><b>127</b></p>  <p>ethyl <i>p</i>-ethoxybenzoate <math>C_{11}H_{14}O_3</math></p>
<p><b>116</b></p>  <p><i>p</i>-nitrobenzaldehyde <math>C_7H_5NO_3</math></p>	<p><b>120</b></p>  <p>4-acetoxybenzoic acid <math>C_9H_8O_4</math></p>	<p><b>124</b></p>  <p>4-aminoacetophenone <math>C_8H_9NO</math></p>	<p><b>128</b></p>  <p>methyl (<i>p</i>-methoxyphenyl)- propionate <math>C_{11}H_{14}O_3</math></p>

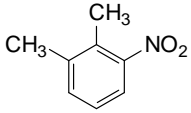
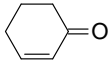
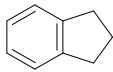
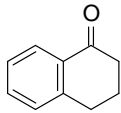
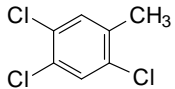
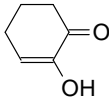
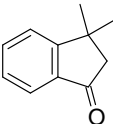
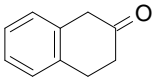
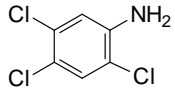
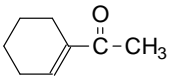
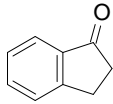
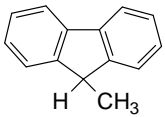
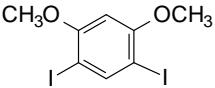
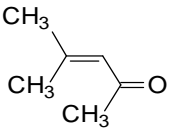
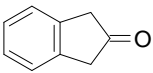
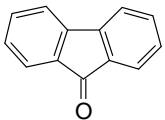
<p><b>129</b></p>  <p><i>N</i>-isopropylbenzylamine <math>C_{10}H_{15}N</math></p>	<p><b>133</b></p>  <p>hydroquinone dipropionate <math>C_{12}H_{14}O_4</math></p>	<p><b>137</b></p>  <p>1,3-dihydroxyphenyl dipropionate <math>C_{12}H_{14}O_4</math></p>	<p><b>141</b></p>  <p>cyclopropyl methyl ketone <math>C_5H_8O</math></p>
<p><b>130</b></p>  <p>methyl 2-methoxy-2- phenylacetate <math>C_{10}H_{12}O_3</math></p>	<p><b>134</b></p>  <p>diethyl terephthalate <math>C_{12}H_{14}O_4</math></p>	<p><b>138</b></p>  <p>dimethyl <i>o</i>-phthalate <math>C_{10}H_{10}O_4</math></p>	<p><b>142</b></p>  <p>cyclopropane carboxylic acid <math>C_4H_6O_2</math></p>
<p><b>131</b></p>  <p>phenyl isocyanate <math>C_7H_5NO</math></p>	<p><b>135</b></p>  <p>diethyl <i>o</i>-phthalate <math>C_{12}H_{14}O_4</math></p>	<p><b>139</b></p>  <p>cycloheptanone <math>C_7H_{12}O</math></p>	<p><b>143</b></p>  <p>benzoylcyclopropane <math>C_{10}H_{10}O</math></p>
<p><b>132</b></p>  <p>phenylacetaldehyde dimethyl acetal <math>C_{10}H_{14}O_2</math></p>	<p><b>136</b></p>  <p>diethyl isophthalate <math>C_{12}H_{14}O_4</math></p>	<p><b>140</b></p>  <p>cycloheptatriene <math>C_7H_8</math></p>	<p><b>144</b></p>  <p>ethyl cyclobutanecarboxylate <math>C_7H_{12}O_2</math></p>

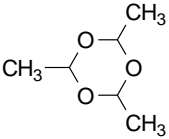
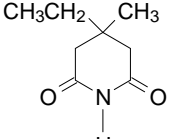
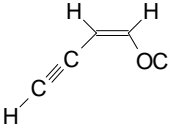
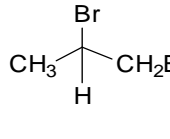
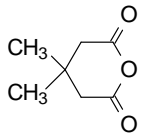
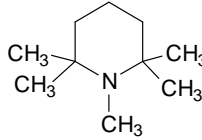
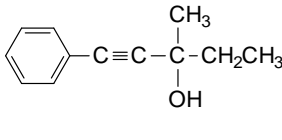
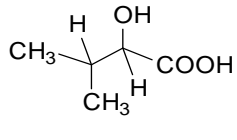
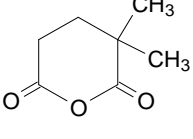
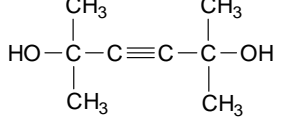
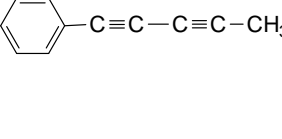
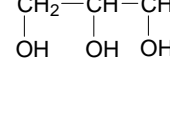
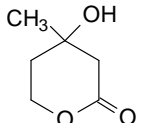
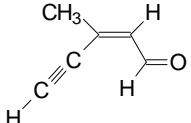
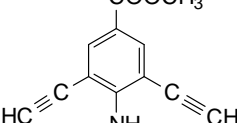
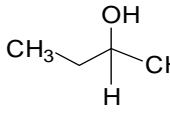
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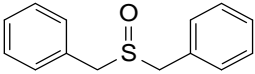
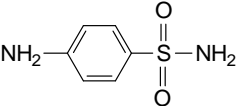
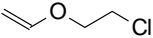
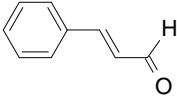
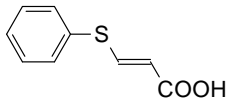
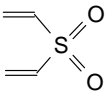
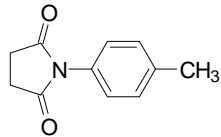
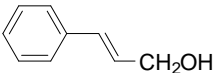
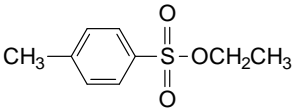
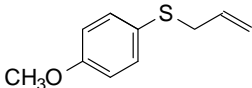
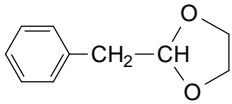
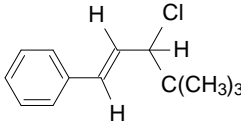
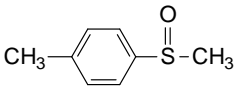
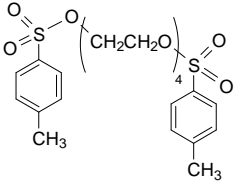
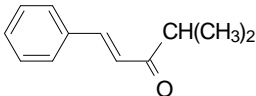
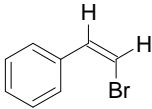
ORGANIC STRUCTURES FROM SPECTRA – 4th EDITION  
L D Field, S Sternhell and J R Kalman

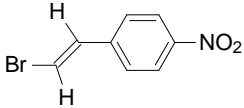
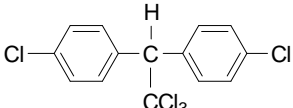
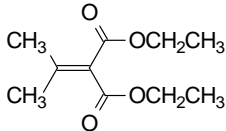
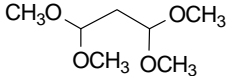
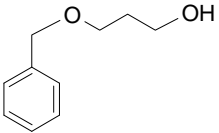
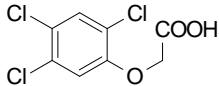
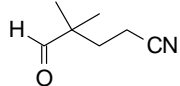
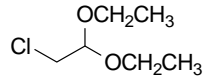
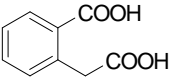
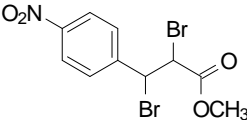
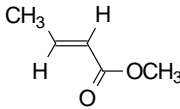
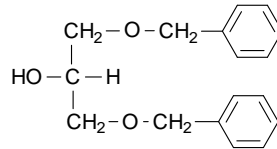
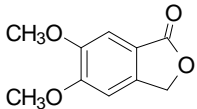
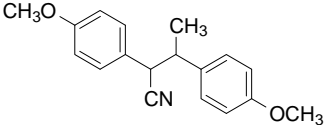
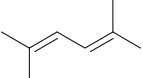

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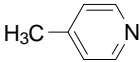
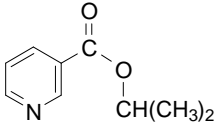
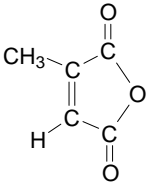
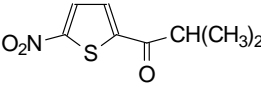
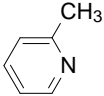
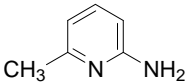
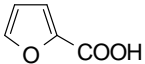
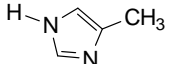
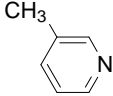
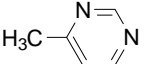
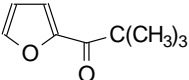
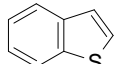
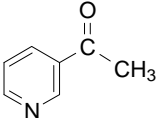
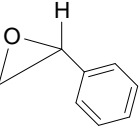
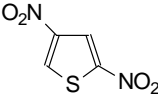
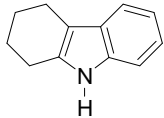
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<p><b>146</b></p>  <p><i>N</i>-methylacetamide</p> <p><math>C_3H_7NO</math></p>	<p><b>150</b></p>  <p>(<i>p</i>-cresyl)methyl phenyl ketone</p> <p><math>C_{15}H_{14}O_2</math></p>	<p><b>154</b></p>  <p>2-bromophenol</p> <p><math>C_6H_5OBr</math></p>	<p><b>158</b></p>  <p>3,5-dibromocumene</p> <p><math>C_9H_{10}Br_2</math></p>
<p><b>147</b></p>  <p>1,4-diaminobutane</p> <p><math>C_4H_{12}N_2</math></p>	<p><b>151</b></p>  <p><i>p</i>-cresyl phenylacetate</p> <p><math>C_{15}H_{14}O_2</math></p>	<p><b>155</b></p>  <p>acetylsalicylic acid (aspirin)</p> <p><math>C_9H_8O_4</math></p>	<p><b>159</b></p>  <p>3-bromo-5-isopropylbenzoic acid</p> <p><math>C_{10}H_{11}O_2Br</math></p>
<p><b>148</b></p>  <p>1,5-diaminopentane</p> <p><math>C_5H_{14}N_2</math></p>	<p><b>152</b></p>  <p>1,3-bis(trichloromethyl)-benzene</p> <p><math>C_8H_4Cl_6</math></p>	<p><b>156</b></p>  <p>2,6-dibromoaniline</p> <p><math>C_6H_5NBr_2</math></p>	<p><b>160</b></p>  <p>piperonal</p> <p><math>C_8H_6O_3</math></p>

<p><b>161</b></p>  <p>3-nitro-<i>o</i>-xylene <math>C_8H_9NO_2</math></p>	<p><b>165</b></p>  <p>2-cyclohexene-1-one <math>C_6H_8O</math></p>	<p><b>169</b></p>  <p>indane <math>C_9H_{10}</math></p>	<p><b>173</b></p>  <p><math>\alpha</math>-tetralone <math>C_{10}H_{10}O</math></p>
<p><b>162</b></p>  <p>2,4,5-trichlorotoluene <math>C_7H_5Cl_3</math></p>	<p><b>166</b></p>  <p>2-hydroxycyclohex-1-en-3-one <math>C_6H_8O_2</math></p>	<p><b>170</b></p>  <p>3,3-dimethylindan-1-one <math>C_{11}H_{12}O</math></p>	<p><b>174</b></p>  <p><math>\beta</math>-tetralone <math>C_{10}H_{10}O</math></p>
<p><b>163</b></p>  <p>2,4,5-trichloroaniline <math>C_6H_4NCl_3</math></p>	<p><b>167</b></p>  <p>1-acetyl-1-cyclohexene <math>C_8H_{12}O</math></p>	<p><b>171</b></p>  <p>1-indanone <math>C_9H_8O</math></p>	<p><b>175</b></p>  <p>9-methylfluorene <math>C_{14}H_{12}</math></p>
<p><b>164</b></p>  <p>4,6-diiodo-1,3-dimethoxybenzene <math>C_8H_8O_2I_2</math></p>	<p><b>168</b></p>  <p>4-methylpent-3-en-2-one (mesityl oxide) <math>C_6H_{10}O</math></p>	<p><b>172</b></p>  <p>2-indanone <math>C_9H_8O</math></p>	<p><b>176</b></p>  <p>fluorenone <math>C_{13}H_8O</math></p>

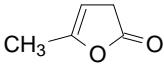
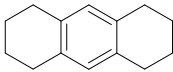
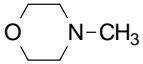
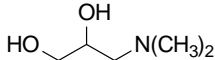
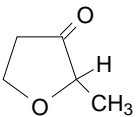
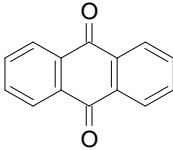
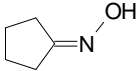
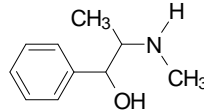

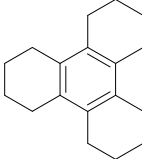
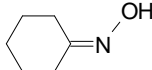
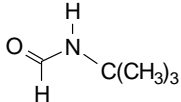
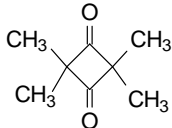
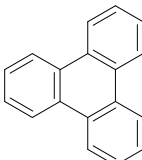
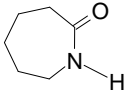
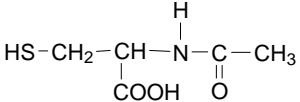
<p><b>177</b></p>  <p>2,4,6-trimethyl- 1,3,5-trioxane C<sub>6</sub>H<sub>12</sub>O<sub>3</sub></p>	<p><b>181</b></p>  <p>4-ethyl-4-methyl-2,6- piperidinedione C<sub>8</sub>H<sub>13</sub>NO<sub>2</sub></p>	<p><b>185</b></p>  <p>(Z)-1-methoxybut- 1-en-4-yne C<sub>5</sub>H<sub>6</sub>O</p>	<p><b>189</b></p>  <p>1,2-dibromopropane C<sub>3</sub>H<sub>6</sub>Br<sub>2</sub></p>
<p><b>178</b></p>  <p>3,3-dimethylglutaric anhydride C<sub>7</sub>H<sub>10</sub>O<sub>3</sub></p>	<p><b>182</b></p>  <p>1,2,2,6,6-pentamethyl- piperidine C<sub>10</sub>H<sub>21</sub>N</p>	<p><b>186</b></p>  <p>3-methyl-1-phenylpent- 1-yn-3-ol C<sub>12</sub>H<sub>14</sub>O</p>	<p><b>190</b></p>  <p>2-hydroxy-3-methylbutyric acid C<sub>5</sub>H<sub>10</sub>O<sub>3</sub></p>
<p><b>179</b></p>  <p>2,2-dimethylglutaric anhydride C<sub>7</sub>H<sub>10</sub>O<sub>3</sub></p>	<p><b>183</b></p>  <p>2,5-dimethyl-3-hexyne- 2,5-diol C<sub>8</sub>H<sub>14</sub>O<sub>2</sub></p>	<p><b>187</b></p>  <p>1-phenyl-1,3-pentadiyne C<sub>11</sub>H<sub>8</sub></p>	<p><b>191</b></p>  <p>glycerol C<sub>3</sub>H<sub>8</sub>O<sub>3</sub></p>
<p><b>180</b></p>  <p>mevalonic lactone C<sub>6</sub>H<sub>10</sub>O<sub>3</sub></p>	<p><b>184</b></p>  <p>(Z)-3-methylpent-2- en-4-ynal C<sub>6</sub>H<sub>6</sub>O</p>	<p><b>188</b></p>  <p>methyl 4-amino-3,5- diethynylbenzoate C<sub>12</sub>H<sub>9</sub>NO<sub>2</sub></p>	<p><b>192</b></p>  <p>2-butanol C<sub>4</sub>H<sub>10</sub>O</p>

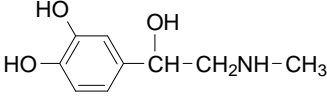
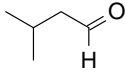
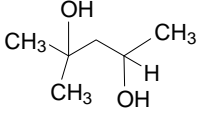
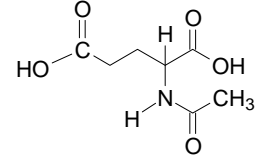
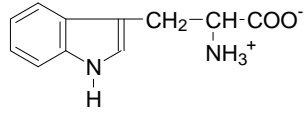
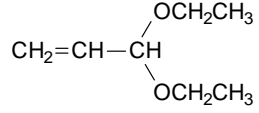
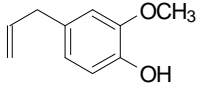
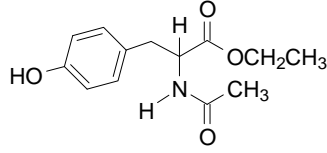
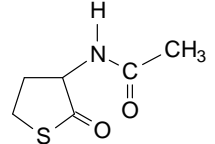
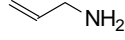
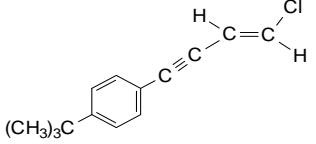

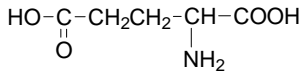
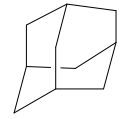
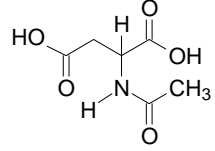

<p><b>193</b></p>  <p>dibenzyl sulfoxide C<sub>14</sub>H<sub>14</sub>OS</p>	<p><b>197</b></p>  <p><i>p</i>-amino- benzenesulfonamide C<sub>6</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S</p>	<p><b>201</b></p>  <p>vinyl 2-chloroethyl ether C<sub>4</sub>H<sub>7</sub>OCl</p>	<p><b>205</b></p>  <p>cinnamaldehyde C<sub>9</sub>H<sub>8</sub>O</p>
<p><b>194</b></p>  <p>(<i>E</i>)-3-(phenylthio)acrylic acid C<sub>9</sub>H<sub>8</sub>O<sub>2</sub>S</p>	<p><b>198</b></p>  <p>divinyl sulfone C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>S</p>	<p><b>202</b></p>  <p><i>N</i>-(<i>p</i>-tolyl)succinimide C<sub>11</sub>H<sub>11</sub>NO<sub>2</sub></p>	<p><b>206</b></p>  <p>cinnamyl alcohol C<sub>9</sub>H<sub>10</sub>O</p>
<p><b>195</b></p>  <p>ethyl <i>p</i>-toluenesulfonate C<sub>9</sub>H<sub>12</sub>O<sub>3</sub>S</p>	<p><b>199</b></p>  <p>allyl <i>p</i>-anisyl thioether C<sub>10</sub>H<sub>12</sub>OS</p>	<p><b>203</b></p>  <p>phenylacetaldehyde ethylene glycol acetal C<sub>10</sub>H<sub>12</sub>O<sub>2</sub></p>	<p><b>207</b></p>  <p>(<i>E</i>)-3-chloro-4,4-dimethyl-1- phenyl-1-pentene C<sub>13</sub>H<sub>17</sub>Cl</p>
<p><b>196</b></p>  <p><i>p</i>-tolyl methyl sulfoxide C<sub>8</sub>H<sub>10</sub>OS</p>	<p><b>200</b></p>  <p>tetraethylene glycol ditosylate C<sub>22</sub>H<sub>30</sub>O<sub>9</sub>S<sub>2</sub></p>	<p><b>204</b></p>  <p>(<i>E</i>)-1-phenyl-4-methyl-1- penten-3-one C<sub>12</sub>H<sub>14</sub>O</p>	<p><b>208</b></p>  <p>(<i>Z</i>)-β-bromostyrene C<sub>8</sub>H<sub>7</sub>Br</p>

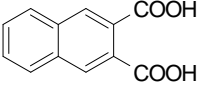
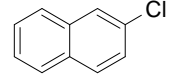
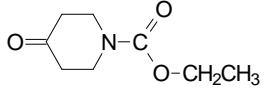
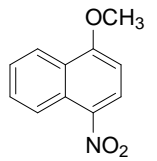
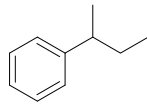
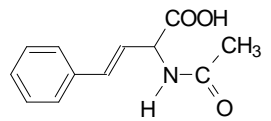
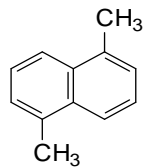
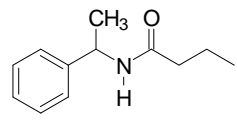
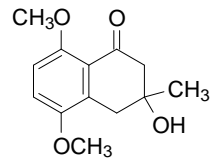
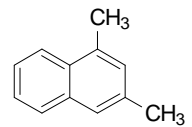
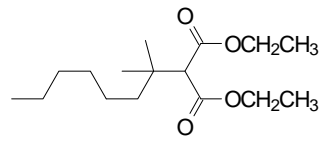
<p><b>209</b></p>  <p>(<i>E</i>)-<i>p</i>-nitro-<math>\beta</math>-bromostyrene <math>C_8H_6BrNO_2</math></p>	<p><b>213</b></p>  <p>1,1-di-(<i>p</i>-chlorophenyl)-2,2,2-trichloroethane (DDT) <math>C_{14}H_9Cl_5</math></p>	<p><b>217</b></p>  <p>diethyl isopropylidene-malonate <math>C_{10}H_{16}O_4</math></p>	<p><b>221</b></p>  <p>malonaldehyde dimethyl acetal <math>C_7H_{16}O_4</math></p>
<p><b>210</b></p>  <p>3-benzyloxy-1-propanol <math>C_{10}H_{14}O_2</math></p>	<p><b>214</b></p>  <p>2,4,5-trichlorophenoxyacetic acid (2,4,5-T) <math>C_8H_5O_3Cl_3</math></p>	<p><b>218</b></p>  <p>4-cyano-2,2-dimethylbutyraldehyde <math>C_7H_{11}NO</math></p>	<p><b>222</b></p>  <p>2-chloroacetaldehyde diethylacetal <math>C_6H_{13}O_2Cl</math></p>
<p><b>211</b></p>  <p>homophthallic acid <math>C_9H_8O_4</math></p>	<p><b>215</b></p>  <p>methyl 2,3-dibromo-3-(<i>p</i>-nitrophenyl)propionate <math>C_{10}H_9NO_4Br_2</math></p>	<p><b>219</b></p>  <p>methyl (<i>E</i>)-3-methylacrylate <math>C_5H_8O_2</math></p>	<p><b>223</b></p>  <p>1,3-dibenzylglycerol <math>C_{17}H_{20}O_3</math></p>
<p><b>212</b></p>  <p>5,6-dimethoxy-2-coumaranone <math>C_{10}H_{10}O_4</math></p>	<p><b>216</b></p>  <p>2,3-di-(<i>p</i>-anisyl)butyronitrile <math>C_{18}H_{19}NO_2</math></p>	<p><b>220</b></p>  <p>2,5-dimethyl-2,4-hexadiene <math>C_8H_{14}</math></p>	<p><b>224</b></p>  <p>pyridine <math>C_5H_5N</math></p>

<p><b>225</b></p>  <p>4-picoline <math>C_6H_7N</math></p>	<p><b>229</b></p>  <p>isopropyl nicotinate <math>C_9H_{11}NO_2</math></p>	<p><b>233</b></p>  <p>citraconic anhydride <math>C_5H_4O_3</math></p>	<p><b>237</b></p>  <p>2-(5-nitrothienyl) isopropyl ketone <math>C_8H_9NO_3S</math></p>
<p><b>226</b></p>  <p>2-picoline <math>C_6H_7N</math></p>	<p><b>230</b></p>  <p>2-methyl-6-aminopyridine <math>C_6H_8N_2</math></p>	<p><b>234</b></p>  <p>2-furoic acid <math>C_5H_4O_3</math></p>	<p><b>238</b></p>  <p>4-methylimidazole <math>C_4H_6N_2</math></p>
<p><b>227</b></p>  <p>3-picoline <math>C_6H_7N</math></p>	<p><b>231</b></p>  <p>4-methylpyrimidine <math>C_5H_6N_2</math></p>	<p><b>235</b></p>  <p>2-furyl <i>t</i>-butyl ketone <math>C_9H_{12}O_2</math></p>	<p><b>239</b></p>  <p>benzothiophene <math>C_8H_6S</math></p>
<p><b>228</b></p>  <p>3-acetylpyridine <math>C_7H_7NO</math></p>	<p><b>232</b></p>  <p>styrene epoxide <math>C_8H_8O</math></p>	<p><b>236</b></p>  <p>2,4-dinitrothiophene <math>C_4H_2N_2O_4S</math></p>	<p><b>240</b></p>  <p>2,3,4,9-tetrahydrocarbazole <math>C_{12}H_{13}N</math></p>



<p><b>241</b></p>  <p><math>\alpha</math>-angelicalactone <math>C_5H_6O_2</math></p>	<p><b>245</b></p>  <p>octahydroanthracene <math>C_{14}H_{18}</math></p>	<p><b>249</b></p>  <p><i>N</i>-methylmorpholine <math>C_5H_{11}NO</math></p>	<p><b>253</b></p>  <p><i>N,N</i>-dimethyl-2,3-dihydroxy- 1-propylamine <math>C_5H_{13}NO_2</math></p>
<p><b>242</b></p>  <p>2-methyl- tetrahydrofuran-3-one <math>C_5H_8O_2</math></p>	<p><b>246</b></p>  <p>anthraquinone <math>C_{14}H_8O_2</math></p>	<p><b>250</b></p>  <p>cyclopentanone oxime <math>C_5H_9NO</math></p>	<p><b>254</b></p>  <p>pseudoephedrine <math>C_{10}H_{15}NO</math></p>
<p><b>243</b></p>  <p>butyrolactone <math>C_4H_6O_2</math></p>	<p><b>247</b></p>  <p>dodecahydrotriphenylene <math>C_{18}H_{24}</math></p>	<p><b>251</b></p>  <p>cyclohexanone oxime <math>C_6H_{11}NO</math></p>	<p><b>255</b></p>  <p><i>t</i>-butylformamide <math>C_5H_{11}NO</math></p>
<p><b>244</b></p>  <p>tetramethyl-1,3- cyclobutanedione <math>C_8H_{12}O_2</math></p>	<p><b>248</b></p>  <p>triphenylene <math>C_{18}H_{12}</math></p>	<p><b>252</b></p>  <p><math>\epsilon</math>-caprolactam <math>C_6H_{11}NO</math></p>	<p><b>256</b></p>  <p><i>N</i>-acetylcysteine <math>C_5H_9NO_3S</math></p>

<p><b>257</b></p>  <p>adrenalin <math>C_9H_{13}NO_3</math></p>	<p><b>261</b></p>  <p>3-methylbutanaldehyde <math>C_5H_{10}O</math></p>	<p><b>265</b></p>  <p>2-methyl-2,4-pentanediol <math>C_6H_{14}O_2</math></p>	<p><b>269</b></p>  <p><i>N</i>-acetylglutamic acid <math>C_7H_{11}NO_5</math></p>
<p><b>258</b></p>  <p>tryptophan <math>C_{11}H_{12}N_2O_2</math></p>	<p><b>262</b></p>  <p>acrolein diethyl acetal <math>C_7H_{14}O_2</math></p>	<p><b>266</b></p>  <p>eugenol <math>C_{10}H_{12}O_2</math></p>	<p><b>270</b></p>  <p><i>N</i>-acetyltyrosine ethyl ester <math>C_{13}H_{17}NO_4</math></p>
<p><b>259</b></p>  <p><i>N</i>-acetylhomocysteine thiolactone <math>C_6H_9NO_2S</math></p>	<p><b>263</b></p>  <p>allylamine <math>C_3H_7N</math></p>	<p><b>267</b></p>  <p><i>E</i>-1-chloro-4-(4-<i>t</i>- butylphenyl)but-1-en-3-yne <math>C_{14}H_{15}Cl</math></p>	<p><b>271</b></p>  <p>2,5-dihydrofuran <math>C_4H_6O</math></p>
<p><b>260</b></p>  <p>glutamic acid <math>C_5H_9NO_4</math></p>	<p><b>264</b></p>  <p>adamantine <math>C_{10}H_{16}</math></p>	<p><b>268</b></p>  <p><i>N</i>-acetylaspartic acid <math>C_6H_9NO_5</math></p>	<p><b>272</b></p>  <p>2,3-dihydrofuran <math>C_4H_6O</math></p>

<p><b>273</b></p>  <p>2,3-naphthalene- dicarboxylic acid <math>C_{12}H_8O_4</math></p>	<p><b>277</b></p>  <p>2-chloronaphthalene <math>C_{10}H_7Cl</math></p>	<p><b>281</b></p>  <p>ethyl 4-piperidone-<i>N</i>- carboxylate <math>C_8H_{13}NO_3</math></p>
<p><b>274</b></p>  <p>1-methoxy-4-nitro- naphthalene <math>C_{11}H_9NO_3</math></p>	<p><b>278</b></p>  <p>sec-butylbenzene <math>C_{10}H_{14}</math></p>	<p><b>282</b></p>  <p><i>N</i>-acetyl-2-amino-4-phenyl- (<i>E</i>)-but-2-enoic acid <math>C_{12}H_{13}NO_3</math></p>
<p><b>275</b></p>  <p>1,5-dimethylnaphthalene <math>C_{12}H_{12}</math></p>	<p><b>279</b></p>  <p><i>N</i>-(1-methyl-1-phenylethyl)- butyramide <math>C_{12}H_{17}NO</math></p>	<p><b>283</b></p>  <p>3-hydroxy-3-methyl-5,8- dimethoxy-1-coumarinone <math>C_{13}H_{16}O_4</math></p>
<p><b>276</b></p>  <p>1,3-dimethylnaphthalene <math>C_{12}H_{12}</math></p>	<p><b>280</b></p>  <p>diethyl 2-(1,1- dimethylheptyl)malonate <math>C_{16}H_{30}O_4</math></p>	

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**Chapter 9.2 – The Analysis of Mixtures Problem 284**

**Problem 284**

<b>Compound</b>	<b>Mole %</b>
ethanol	57
bromoethane	43

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**Problem 285**

<b>Compound</b>	<b>Mole %</b>
benzene	15
diethyl ether	46
dichloromethane	39

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**Problem 286**

<b>Compound</b>	<b>Mole %</b>
benzene	24
ethyl acetate	59
dioxane	17

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**Problem 287**

<b>Compound</b>	<b>Mole %</b>
ethanol	41
bromoethane	59

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Problem 288

Compound	Mole %
benzene	13
diethyl ether	22
dichloromethane	65

---

Problem 290

Compound	Mole %
fluorene	75
fluorenone	25

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Problem 289

Compound	Mole %
benzene	23
ethyl acetate	51
dioxane	26

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Problem 291

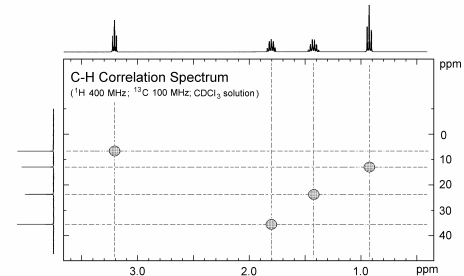
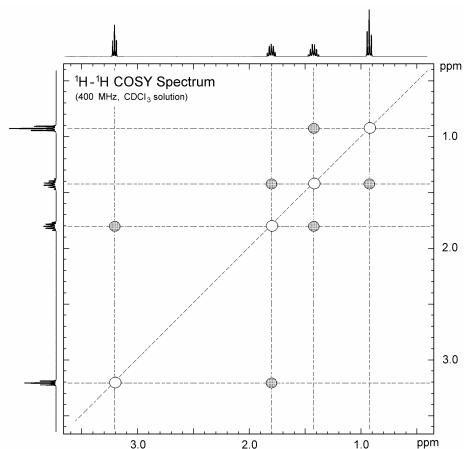
Compound	Mole %
4-nitroanisole	38
2-nitroanisole	62

Chapter 9.3 – Problems in 2D NMR

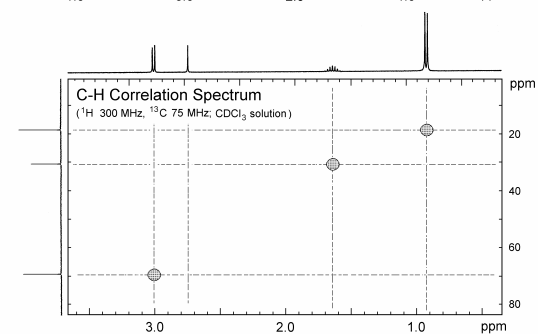
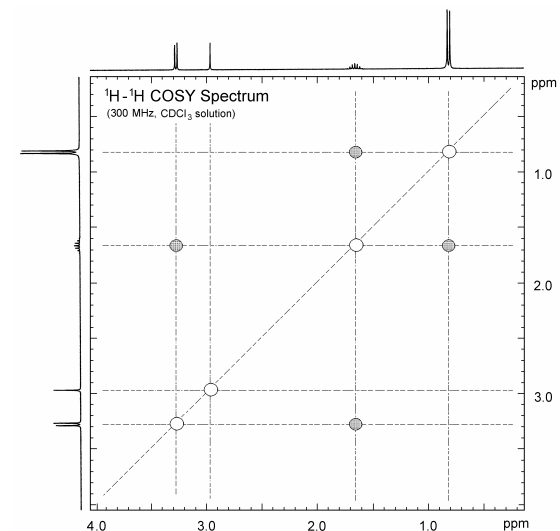
Problem 292 1-propanol

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

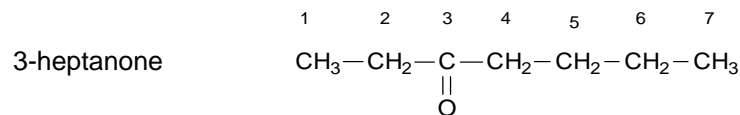
Problem 293 1-iodobutane



Problem 294 isobutanol



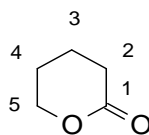
Problem 295



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

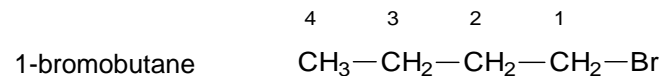
Problem 296

$\delta$ -valerolactone



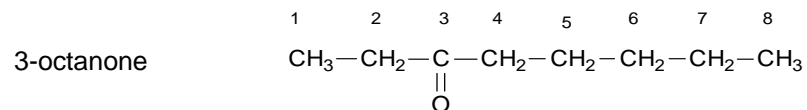
Proton	Chemical Shift ( $\delta$ ) in ppm	Carbon	Chemical Shift ( $\delta$ ) in ppm
		C1	170.0
H2	2.08	C2	29.9
H3	1.16	C3	22.2
H4	1.08	C4	19.0
H5	3.71	C5	68.8

Problem 297



Proton	Chemical Shift ( $\delta$ ) in ppm	Carbon	Chemical Shift ( $\delta$ ) 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

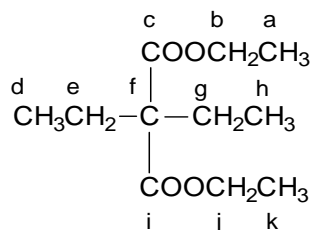
Problem 298



Proton	Chemical Shift ( $\delta$ ) in ppm	Carbon	Chemical Shift ( $\delta$ ) 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

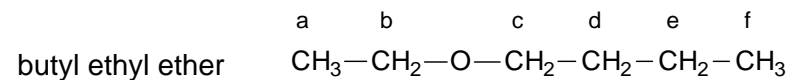
Problem 299

diethyl diethylmalonate



Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
H <sub>a</sub>	1.19	C <sub>a</sub>	14.0
H <sub>b</sub>	4.13	C <sub>b</sub>	60.8
		C <sub>c</sub>	171.9
H <sub>d</sub>	0.76	C <sub>d</sub>	8.1
H <sub>e</sub>	1.88	C <sub>e</sub>	24.5
		C <sub>f</sub>	58.0
H <sub>g</sub>	1.88	C <sub>g</sub>	24.5
H <sub>h</sub>	0.76	C <sub>h</sub>	8.1
		C <sub>i</sub>	171.9
H <sub>j</sub>	4.13	C <sub>j</sub>	60.8
H <sub>k</sub>	1.19	C <sub>k</sub>	14.0

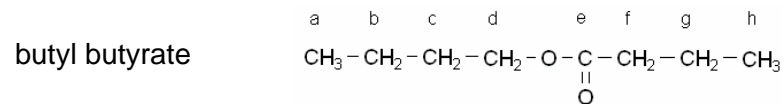
Problem 300



Proton	Chemical Shift (δ) in ppm	Carbon	Chemical Shift (δ) in ppm
H <sub>a</sub>	1.11	C <sub>a</sub>	15.0
H <sub>b</sub>	3.29	C <sub>b</sub>	66.0
H <sub>c</sub>	3.27	C <sub>c</sub>	70.1
H <sub>d</sub>	1.52	C <sub>d</sub>	32.1
H <sub>e</sub>	1.36	C <sub>e</sub>	19.4
H <sub>f</sub>	0.87	C <sub>f</sub>	13.5

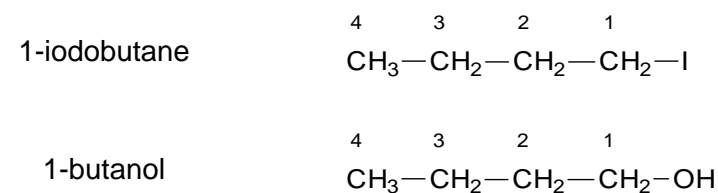


Problem 301



Proton	Chemical Shift ( $\delta$ ) in ppm	Carbon	Chemical Shift ( $\delta$ ) in ppm
H <sub>a</sub>	0.75	C <sub>a</sub>	13.9
H <sub>b</sub>	1.19	C <sub>b</sub>	19.5
H <sub>c</sub>	1.40	C <sub>c</sub>	31.2
H <sub>d</sub>	3.97	C <sub>d</sub>	64.0
		C <sub>e</sub>	172.8
H <sub>f</sub>	2.08	C <sub>f</sub>	36.2
H <sub>g</sub>	1.52	C <sub>g</sub>	19.0
H <sub>h</sub>	0.79	C <sub>h</sub>	13.9

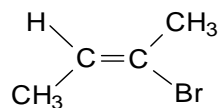
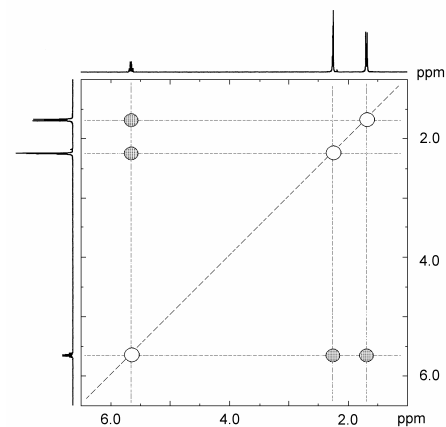
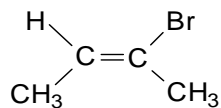
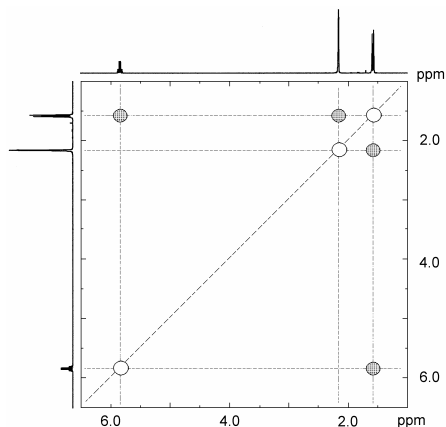
Problem 302



1-iodobutane	<sup>1</sup> H Chemical Shift ( $\delta$ ) in ppm	1-butanol	<sup>1</sup> H Chemical Shift ( $\delta$ ) 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

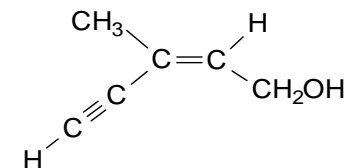
Problem 303

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



Problem 304

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

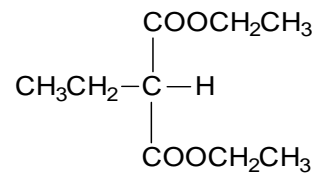


Problem 305

Proton	Chemical Shift ( $\delta$ ) in ppm
H2	8.22
H3	7.53
H4	8.10
H5	7.95
H6	7.62
H7	7.71
H8	8.56

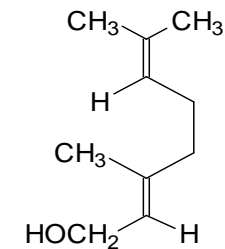
Problem 306

ethyl diethylmalonate



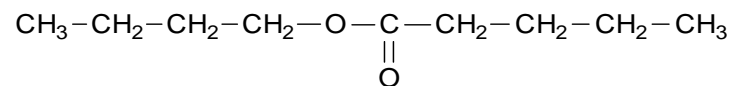
Problem 309

geraniol



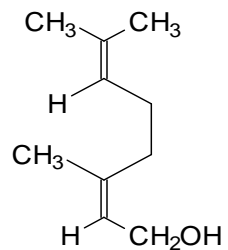
Problem 307

butyl  
valerate




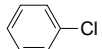
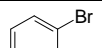
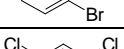
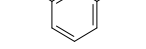
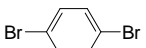
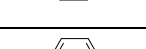
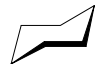


Problem 308

nerol

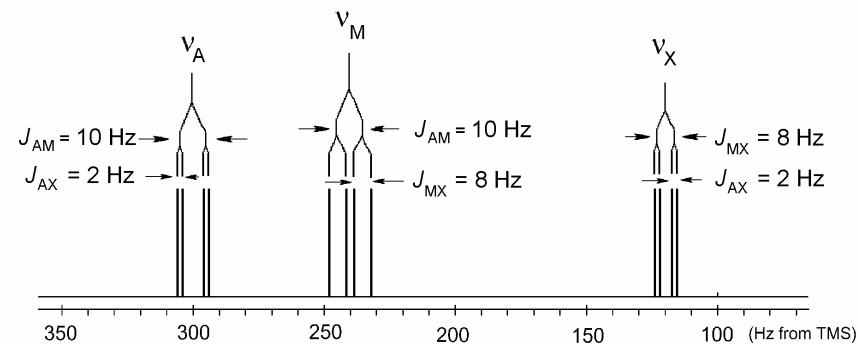


Chapter 9.4 – Analysis of NMR Spectra

Problem 310

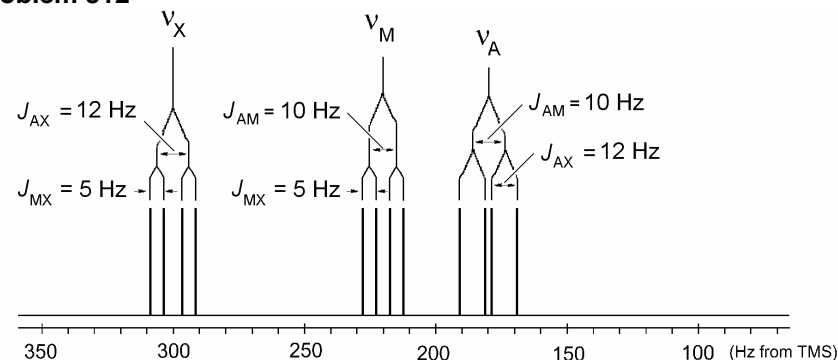
Structure	Number of 1H environments	Number of 13C environments
<chem>CH3-CO-CH2CH2CH3</chem>	4	5
<chem>CH3CH2-CO-CH2CH3</chem>	2	3
<chem>CH2=CHCH2CH3</chem>	5	4
<i>cis</i> - <chem>CH3CH=CHCH3</chem>	2	2
<i>trans</i> - <chem>CH3CH=CHCH3</chem>	2	2
	1	1
	3	4
	2	3
	3	4
	1	2
	2	4
	5	7
 <b>slow chair-chair</b>	2	1
 <b>fast chair-chair</b>	1	1
 <b>rigid</b>	7	4

Problem 311



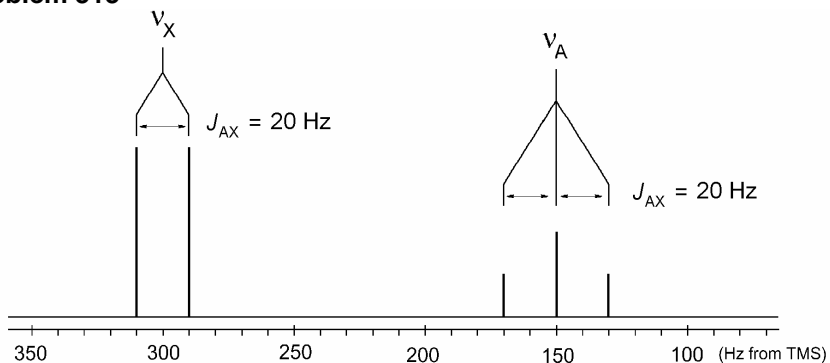
Chemical Shifts  $\delta_A = 300 \text{ Hz} / 60 \text{ MHz} = 5.0 \text{ ppm}$   
 $\delta_M = 240 \text{ Hz} / 60 \text{ MHz} = 4.0 \text{ ppm}$   
 $\delta_X = 120 \text{ Hz} / 60 \text{ MHz} = 2.0 \text{ ppm}$

Problem 312



Chemical Shifts  $\delta_A = 180 \text{ Hz} / 200 \text{ MHz} = 0.90 \text{ ppm}$   
 $\delta_M = 220 \text{ Hz} / 200 \text{ MHz} = 1.22 \text{ ppm}$   
 $\delta_X = 300 \text{ Hz} / 200 \text{ MHz} = 1.50 \text{ ppm}$

Problem 313



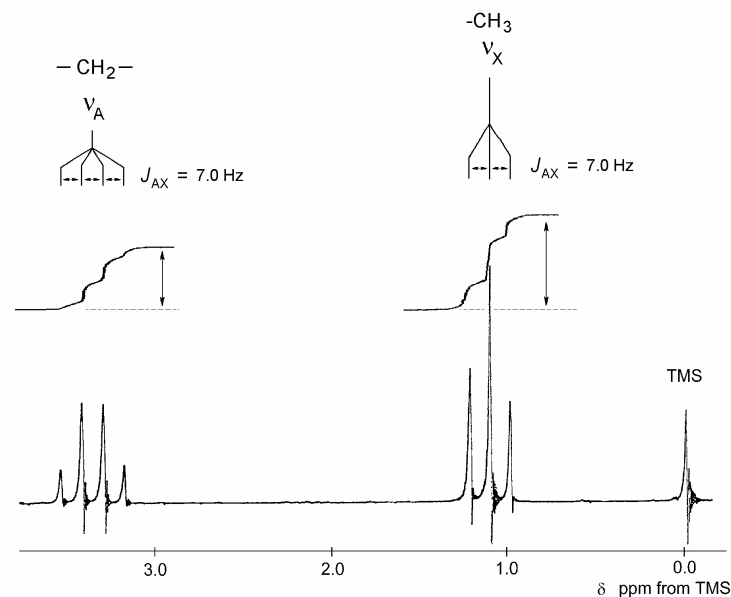
Chemical Shifts

$$\delta_A = 150 \text{ Hz} / 400 \text{ MHz} = 0.375 \text{ ppm}$$

$$\delta_X = 300 \text{ Hz} / 400 \text{ MHz} = 0.750 \text{ ppm}$$

Problem 314

Spin System  $A_2X_3$



Chemical Shifts

$$\delta_A = 3.36 \text{ ppm} = 3.36 \times 60 = 202 \text{ Hz from TMS}$$

$$\delta_X = 1.11 \text{ ppm} = 1.11 \times 60 = 67 \text{ Hz from TMS}$$

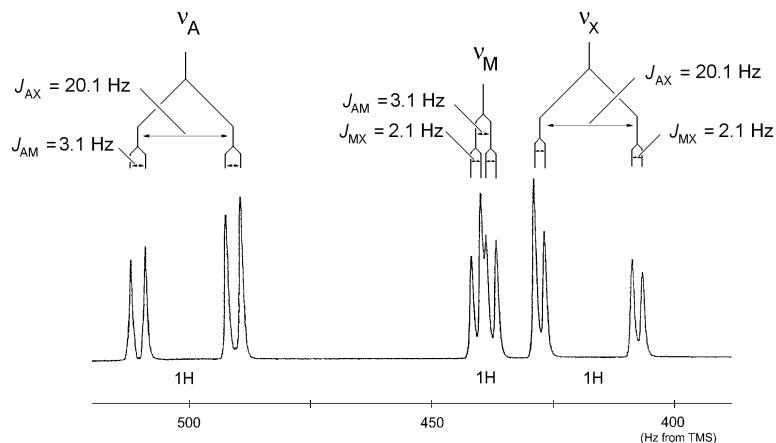
1st Order Analysis

$$\Delta\nu_{AX} = \nu_A - \nu_X = 202 - 67 = 135 \text{ Hz}$$

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

This ratio is much greater than 3 so a 1<sup>st</sup> order analysis is justified.

Problem 315 Spin System AMX



Chemical Shifts

$$\begin{aligned}\delta_A &= 501 \text{ Hz} / 100 \text{ MHz} = 5.01 \text{ ppm} \\ \delta_M &= 439 \text{ Hz} / 100 \text{ MHz} = 4.39 \text{ ppm} \\ \delta_X &= 408 \text{ Hz} / 100 \text{ MHz} = 4.08 \text{ ppm}\end{aligned}$$

Coupling constants

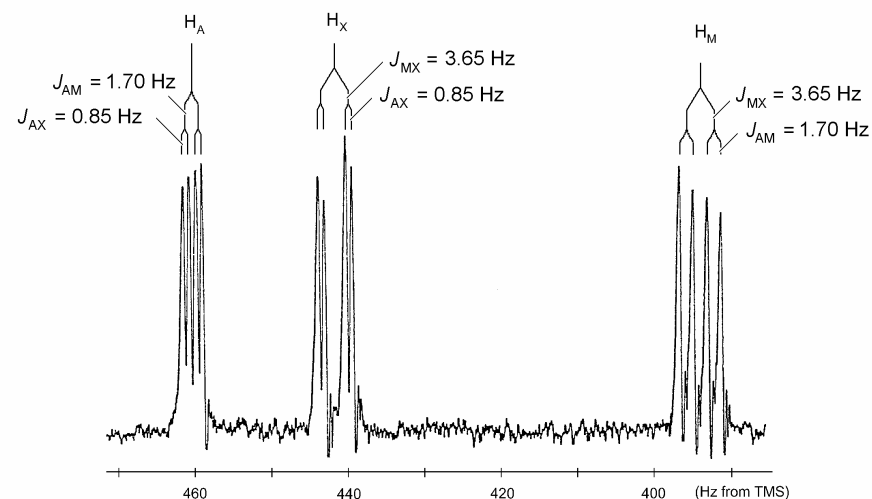
$$\begin{aligned}J_{AM} &= 3.1 \text{ Hz} \\ J_{AX} &= 20.1 \text{ Hz} \\ J_{MX} &= 1.1 \text{ Hz}\end{aligned}$$

1st Order Analysis

$$\begin{aligned}\Delta\nu_{AM} &= \nu_A - \nu_M = 501 - 439 = 62 \text{ Hz} \\ \Delta\nu_{AX} &= \nu_A - \nu_X = 501 - 408 = 93 \text{ Hz} \\ \Delta\nu_{MX} &= \nu_M - \nu_X = 439 - 408 = 31 \text{ Hz} \\ \Delta\nu_{AM} / J_{AM} &= 62 / 3.1 = 20.0 \\ \Delta\nu_{AX} / J_{AX} &= 93 / 20.1 = 4.6 \\ \Delta\nu_{MX} / J_{MX} &= 31 / 2.1 = 14.7\end{aligned}$$

All ratios are greater than 3 so a 1<sup>st</sup> order analysis is justified.

Problem 316 Spin System AMX



Chemical Shifts

$$\begin{aligned}\delta_A &= 460 \text{ Hz} / 60 \text{ MHz} = 7.67 \text{ ppm} \\ \delta_X &= 442 \text{ Hz} / 60 \text{ MHz} = 7.37 \text{ ppm} \\ \delta_M &= 394 \text{ Hz} / 60 \text{ MHz} = 6.57 \text{ ppm}\end{aligned}$$

Coupling constants

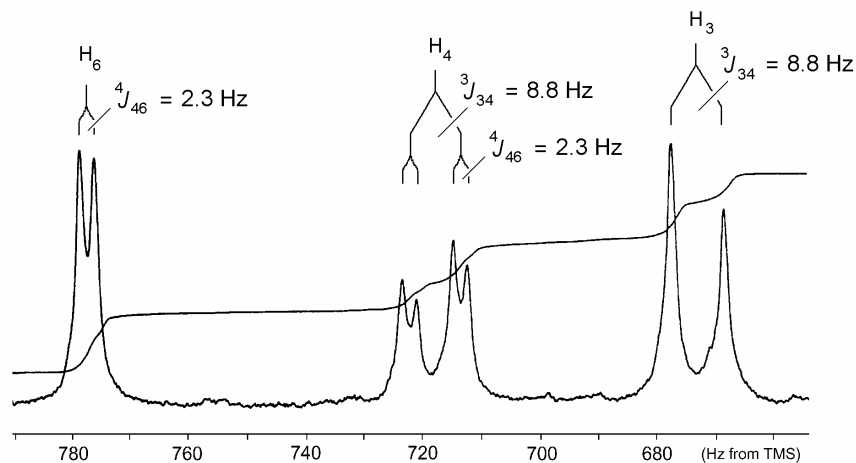
$$\begin{aligned}J_{AM} &= 1.70 \text{ Hz} \\ J_{AX} &= 0.85 \text{ Hz} \\ J_{MX} &= 3.65 \text{ Hz}\end{aligned}$$

1st Order Analysis

$$\begin{aligned}\Delta\nu_{AM} &= \nu_A - \nu_M = 460 - 394 = 66 \text{ Hz} \\ \Delta\nu_{AX} &= \nu_A - \nu_X = 460 - 442 = 18 \text{ Hz} \\ \Delta\nu_{MX} &= \nu_M - \nu_X = 442 - 394 = 48 \text{ Hz} \\ \Delta\nu_{AM} / J_{AM} &= 66 / 1.7 = 38.8 \\ \Delta\nu_{AX} / J_{AX} &= 18 / 0.85 = 21.2 \\ \Delta\nu_{MX} / J_{MX} &= 48 / 3.65 = 13.2\end{aligned}$$

All ratios are greater than 3 so a 1<sup>st</sup> order analysis is justified.

Problem 317 Spin System AMX



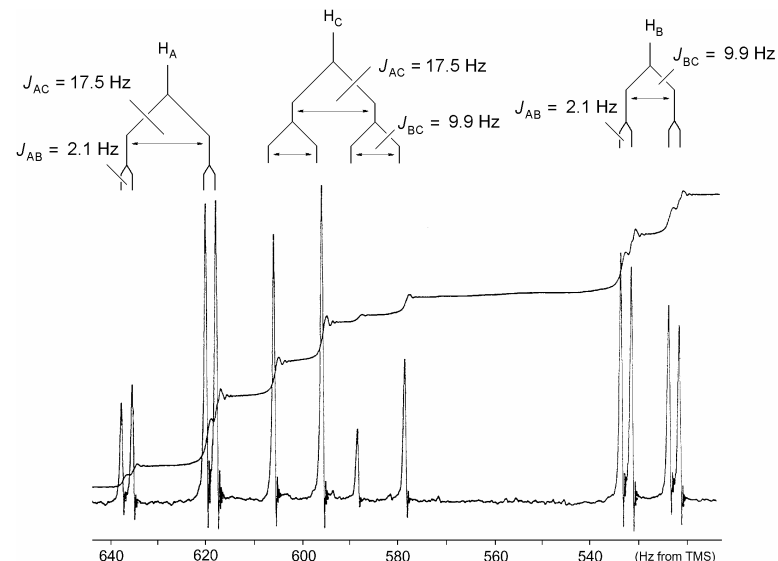
**Chemical Shifts**  
 $\delta_3 = 673 \text{ Hz} / 100 \text{ MHz} = 6.73 \text{ ppm}$   
 $\delta_4 = 719 \text{ Hz} / 100 \text{ MHz} = 7.19 \text{ ppm}$   
 $\delta_6 = 777 \text{ Hz} / 100 \text{ MHz} = 7.77 \text{ ppm}$

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

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

All ratios are greater than 3 so a 1<sup>st</sup> order analysis is justified.

Problem 318 Spin System AMX



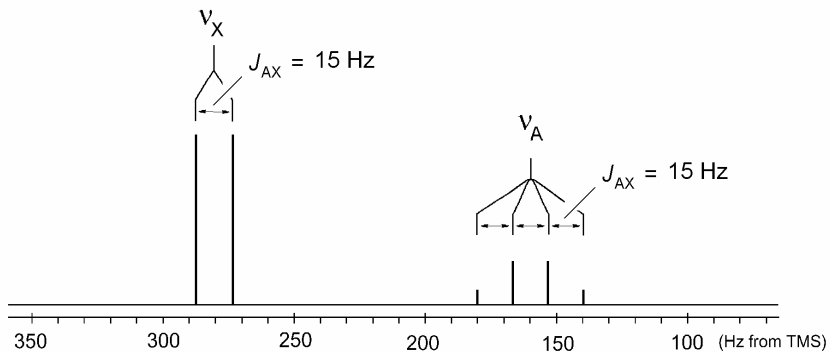
**Chemical Shifts**  
 $\delta_A = 628 \text{ Hz} / 100 \text{ MHz} = 6.28 \text{ ppm}$   
 $\delta_B = 527 \text{ Hz} / 100 \text{ MHz} = 5.27 \text{ ppm}$   
 $\delta_C = 592 \text{ Hz} / 100 \text{ MHz} = 5.92 \text{ ppm}$

**Coupling constants**  $J_{AB} = 2.1 \text{ Hz}$ ;  $J_{AC} = 17.5 \text{ Hz}$ ;  $J_{BC} = 9.9 \text{ Hz}$

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

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

Problem 319 Spin System AX<sub>3</sub>

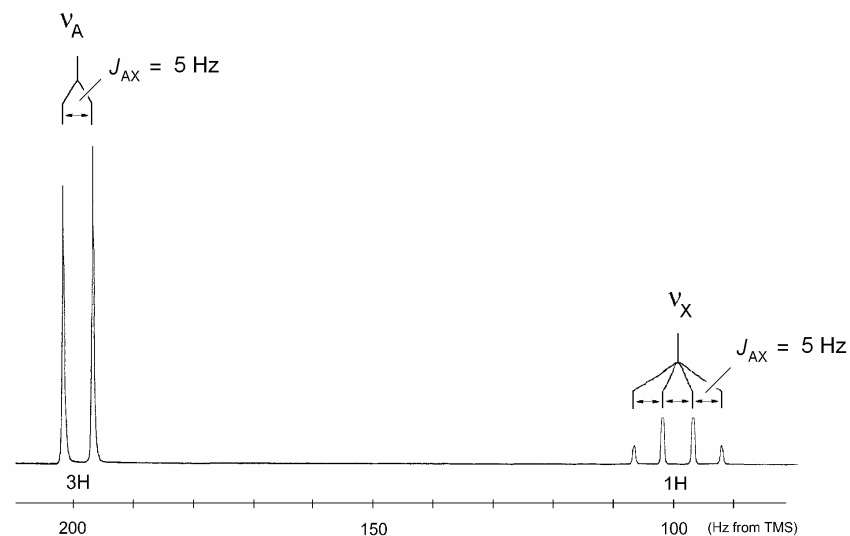


Chemical Shifts

$$\delta_A = 160 \text{ Hz} / 60 \text{ MHz} = 2.67 \text{ ppm}$$

$$\delta_X = 280 \text{ Hz} / 60 \text{ MHz} = 4.67 \text{ ppm}$$

Problem 320 Spin System AX<sub>3</sub>



Chemical Shifts

$$\delta_A = 199 \text{ Hz} / 100 \text{ MHz} = 1.99 \text{ ppm}$$

$$\delta_X = 99 \text{ Hz} / 100 \text{ MHz} = 0.99 \text{ ppm}$$

Coupling constants

$$J_{AX} = 5 \text{ Hz}$$

1st Order Analysis

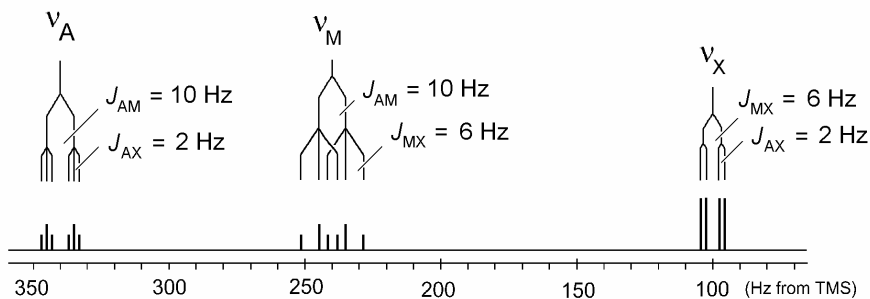
$$\Delta\nu_{AX} = \nu_A - \nu_X = 199 - 99 = 100 \text{ Hz}$$

$$\Delta\nu_{AX} / J_{AX} = 100 / 5 = 20.0$$

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



Problem 321 4 Spin System AMX<sub>2</sub>



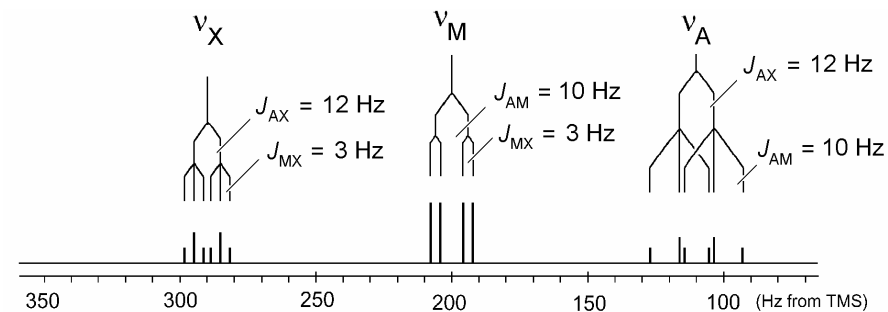
Chemical Shifts

$$\delta_A = 340 \text{ Hz} / 60 \text{ MHz} = 5.67 \text{ ppm}$$

$$\delta_M = 240 \text{ Hz} / 60 \text{ MHz} = 4.00 \text{ ppm}$$

$$\delta_X = 100 \text{ Hz} / 60 \text{ MHz} = 1.67 \text{ ppm}$$

Problem 322 4 Spin System AM<sub>2</sub>X



Chemical Shifts

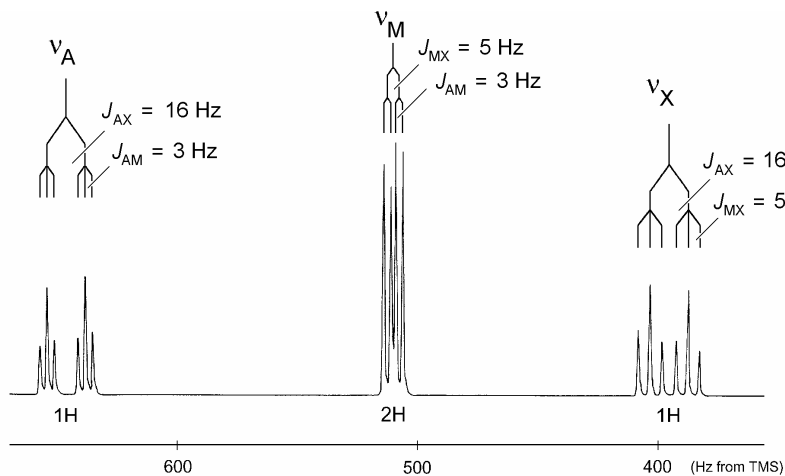
$$\delta_A = 110 \text{ Hz} / 60 \text{ MHz} = 1.83 \text{ ppm}$$

$$\delta_M = 200 \text{ Hz} / 60 \text{ MHz} = 3.33 \text{ ppm}$$

$$\delta_X = 290 \text{ Hz} / 60 \text{ MHz} = 4.83 \text{ ppm}$$

Problem 323 4 Spin System

AM<sub>2</sub>X



Chemical Shifts

$$\delta_A = 646 \text{ Hz} / 100 \text{ MHz} = 6.46 \text{ ppm}$$

$$\delta_M = 510 \text{ Hz} / 100 \text{ MHz} = 5.10 \text{ ppm}$$

$$\delta_X = 395 \text{ Hz} / 100 \text{ MHz} = 3.95 \text{ ppm}$$

Coupling constants

$$J_{AM} = 3 \text{ Hz}; J_{AX} = 16 \text{ Hz}; J_{MX} = 5 \text{ Hz};$$

1st Order Analysis

$$\Delta\nu_{AX} = \nu_A - \nu_X = 646 - 395 = 251 \text{ Hz}$$

$$\Delta\nu_{AM} = \nu_A - \nu_M = 646 - 510 = 136 \text{ Hz}$$

$$\Delta\nu_{MX} = \nu_M - \nu_X = 510 - 395 = 115 \text{ Hz}$$

$$\Delta\nu_{AX} / J_{AX} = 251 / 16 = 15.7$$

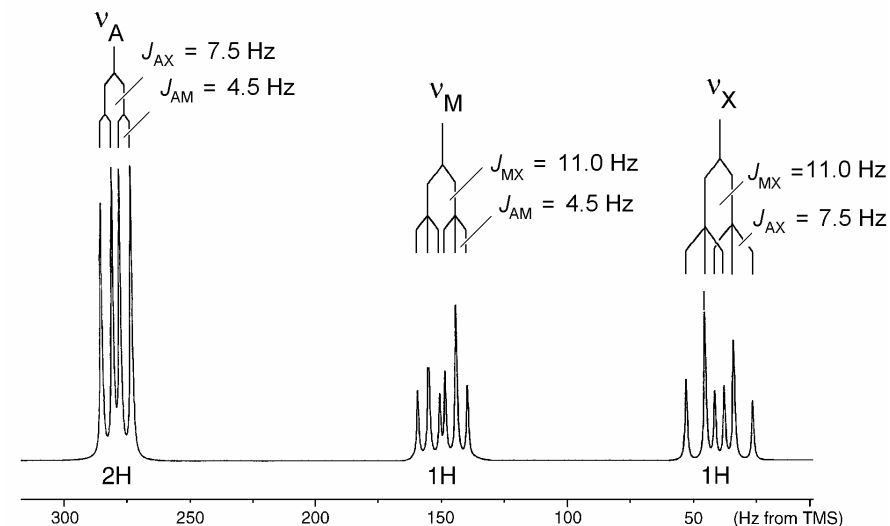
$$\Delta\nu_{AM} / J_{AM} = 136 / 3 = 45.3$$

$$\Delta\nu_{MX} / J_{MX} = 115 / 5 = 23.0$$

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

Problem 324 4 Spin System

A<sub>2</sub>MX



Chemical Shifts

$$\delta_A = 279 \text{ Hz} / 100 \text{ MHz} = 2.79 \text{ ppm}$$

$$\delta_M = 149 \text{ Hz} / 100 \text{ MHz} = 1.49 \text{ ppm}$$

$$\delta_X = 39 \text{ Hz} / 100 \text{ MHz} = 0.39 \text{ ppm}$$

Coupling constants

$$J_{AM} = 4.5 \text{ Hz}; J_{AX} = 7.5 \text{ Hz}; J_{MX} = 11.0 \text{ Hz};$$

1st Order Analysis

$$\Delta\nu_{AX} = \nu_A - \nu_X = 279 - 39 = 240 \text{ Hz}$$

$$\Delta\nu_{AM} = \nu_A - \nu_M = 279 - 149 = 130 \text{ Hz}$$

$$\Delta\nu_{MX} = \nu_M - \nu_X = 149 - 39 = 110 \text{ Hz}$$

$$\Delta\nu_{AX} / J_{AX} = 240 / 7.5 = 32.0$$

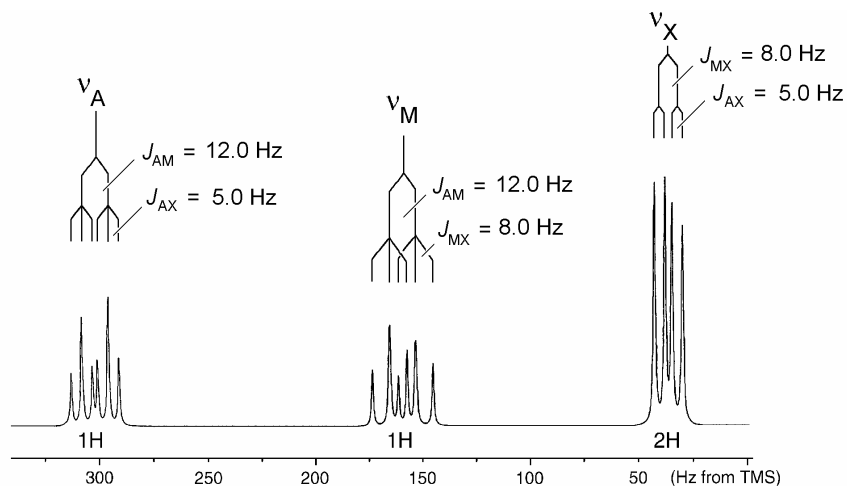
$$\Delta\nu_{AM} / J_{AM} = 130 / 4.5 = 28.9$$

$$\Delta\nu_{MX} / J_{MX} = 110 / 11 = 10.0$$

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

Problem 325 4 Spin System

AMX<sub>2</sub>



Chemical Shifts

$$\delta_A = 302 \text{ Hz} / 100 \text{ MHz} = 3.02 \text{ ppm}$$

$$\delta_M = 160 \text{ Hz} / 100 \text{ MHz} = 1.60 \text{ ppm}$$

$$\delta_X = 37 \text{ Hz} / 100 \text{ MHz} = 0.37 \text{ ppm}$$

Coupling constants

$$J_{AM} = 12.0 \text{ Hz}; J_{AX} = 5.0 \text{ Hz}; J_{MX} = 8.0 \text{ Hz};$$

1st Order Analysis

$$\Delta\nu_{AX} = \nu_A - \nu_X = 302 - 37 = 265 \text{ Hz}$$

$$\Delta\nu_{AM} = \nu_A - \nu_M = 302 - 160 = 142 \text{ Hz}$$

$$\Delta\nu_{MX} = \nu_M - \nu_X = 160 - 37 = 123 \text{ Hz}$$

$$\Delta\nu_{AX} / J_{AX} = 265 / 5.0 = 53.0$$

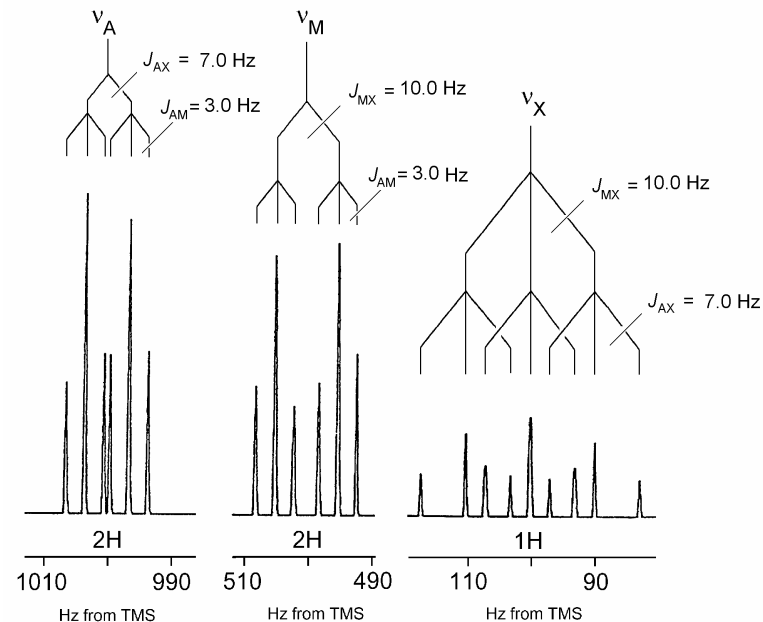
$$\Delta\nu_{AM} / J_{AM} = 142 / 12.0 = 11.8$$

$$\Delta\nu_{MX} / J_{MX} = 123 / 8.0 = 15.4$$

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

Problem 326 5 Spin System

A<sub>2</sub>M<sub>2</sub>X



Chemical Shifts

$$\delta_A = 1000 \text{ Hz} / 200 \text{ MHz} = 5.0 \text{ ppm}$$

$$\delta_M = 500 \text{ Hz} / 200 \text{ MHz} = 2.5 \text{ ppm}$$

$$\delta_X = 100 \text{ Hz} / 200 \text{ MHz} = 0.5 \text{ ppm}$$

Coupling constants

$$J_{AM} = 3.0 \text{ Hz}; J_{AX} = 7.0 \text{ Hz}; J_{MX} = 10.0 \text{ Hz};$$

1st Order Analysis

$$\Delta\nu_{AX} = \nu_A - \nu_X = 1000 - 100 = 900 \text{ Hz}$$

$$\Delta\nu_{AM} = \nu_A - \nu_M = 1000 - 500 = 500 \text{ Hz}$$

$$\Delta\nu_{MX} = \nu_M - \nu_X = 500 - 100 = 400 \text{ Hz}$$

$$\Delta\nu_{AX} / J_{AX} = 900 / 7.0 = 128.6$$

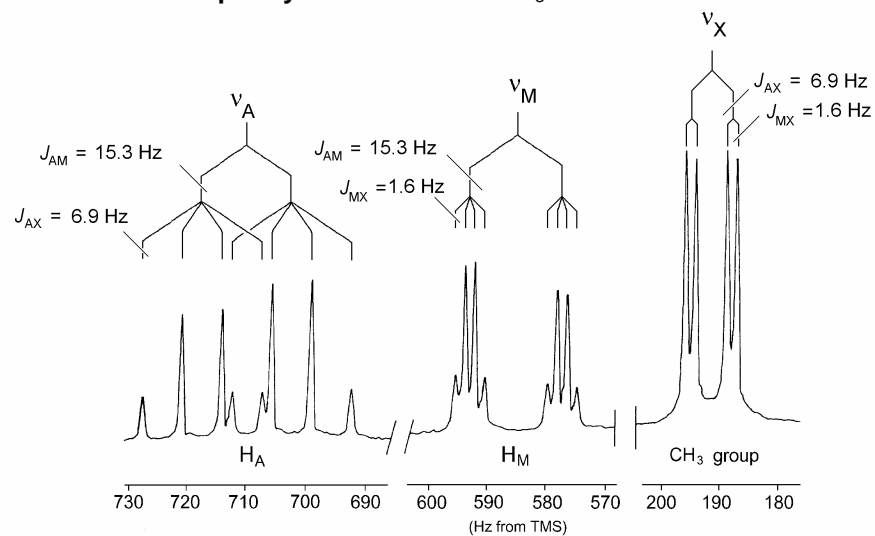
$$\Delta\nu_{AM} / J_{AM} = 500 / 3.0 = 166.7$$

$$\Delta\nu_{MX} / J_{MX} = 400 / 10.0 = 40.0$$

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

Problem 327 5 Spin System

AMX<sub>3</sub>



Chemical Shifts

$$\delta_A = 710 \text{ Hz} / 100 \text{ MHz} = 7.10 \text{ ppm}$$

$$\delta_M = 585 \text{ Hz} / 100 \text{ MHz} = 5.85 \text{ ppm}$$

$$\delta_X = 192 \text{ Hz} / 100 \text{ MHz} = 1.92 \text{ ppm}$$

Coupling constants

$$J_{AM} = 15.3 \text{ Hz}; J_{AX} = 6.9 \text{ Hz}; J_{MX} = 1.6 \text{ Hz};$$

1st Order Analysis

$$\Delta\nu_{AX} = \nu_A - \nu_X = 710 - 192 = 518 \text{ Hz}$$

$$\Delta\nu_{AM} = \nu_A - \nu_M = 710 - 585 = 125 \text{ Hz}$$

$$\Delta\nu_{MX} = \nu_M - \nu_X = 585 - 192 = 393 \text{ Hz}$$

$$\Delta\nu_{AX} / J_{AX} = 518 / 6.9 = 84.7$$

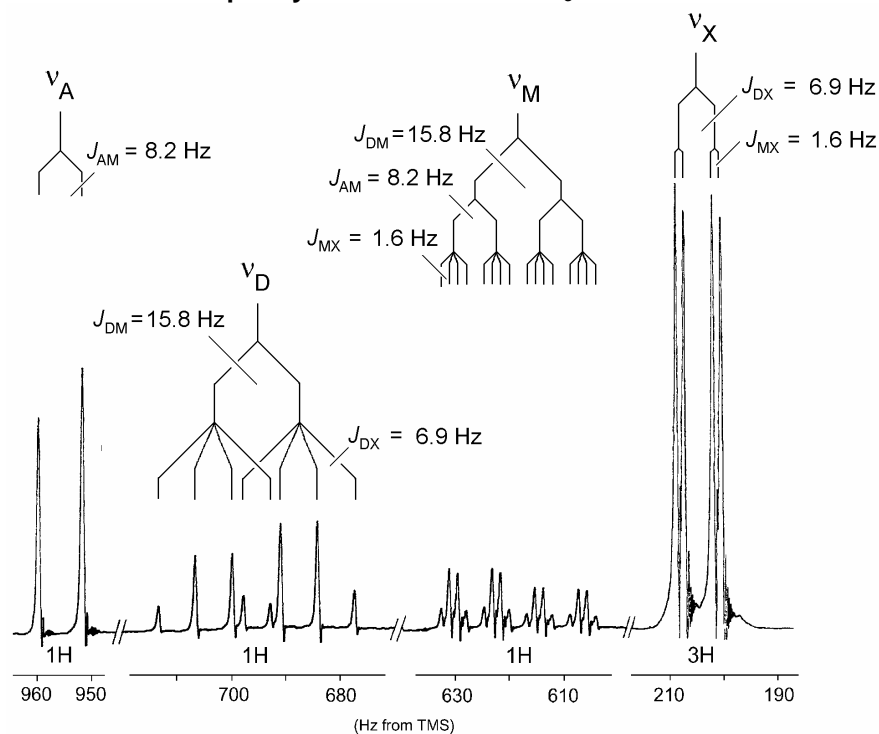
$$\Delta\nu_{AM} / J_{AM} = 125 / 15.3 = 8.2$$

$$\Delta\nu_{MX} / J_{MX} = 393 / 1.6 = 245.6$$

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

Problem 328 5 Spin System

ADMX<sub>3</sub>



Chemical Shifts

$$\begin{aligned}\delta_A &= 956 \text{ Hz} / 100 \text{ MHz} = 9.56 \text{ ppm}; \\ \delta_D &= 695 \text{ Hz} / 100 \text{ MHz} = 6.95 \text{ ppm}; \\ \delta_M &= 619 \text{ Hz} / 100 \text{ MHz} = 6.19 \text{ ppm}; \\ \delta_X &= 205 \text{ Hz} / 100 \text{ MHz} = 2.05 \text{ ppm};\end{aligned}$$

Coupling constants

$$\begin{aligned}J_{AD} &= < 1 \text{ Hz}; J_{AM} = 8.2 \text{ Hz}; J_{AX} = < 1 \text{ Hz}; \\ J_{DM} &= 15.8 \text{ Hz}; J_{DX} = 6.9 \text{ Hz}; J_{MX} = 1.6 \text{ Hz};\end{aligned}$$

1st Order Analysis

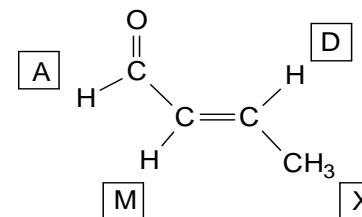
$$\begin{aligned}\Delta\nu_{AD} &= \nu_A - \nu_D = 956 - 695 = 261 \text{ Hz} \\ \Delta\nu_{AM} &= \nu_A - \nu_M = 956 - 619 = 337 \text{ Hz} \\ \Delta\nu_{AX} &= \nu_A - \nu_X = 956 - 205 = 751 \text{ Hz} \\ \Delta\nu_{DM} &= \nu_D - \nu_M = 695 - 619 = 76 \text{ Hz} \\ \Delta\nu_{DX} &= \nu_D - \nu_X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

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

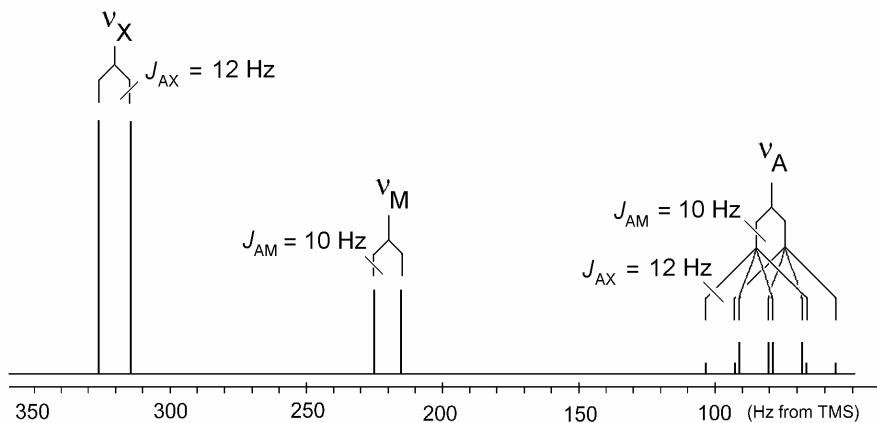
All ratios are significantly greater than 3 so a 1<sup>st</sup> order analysis is justified.

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<sub>3</sub>



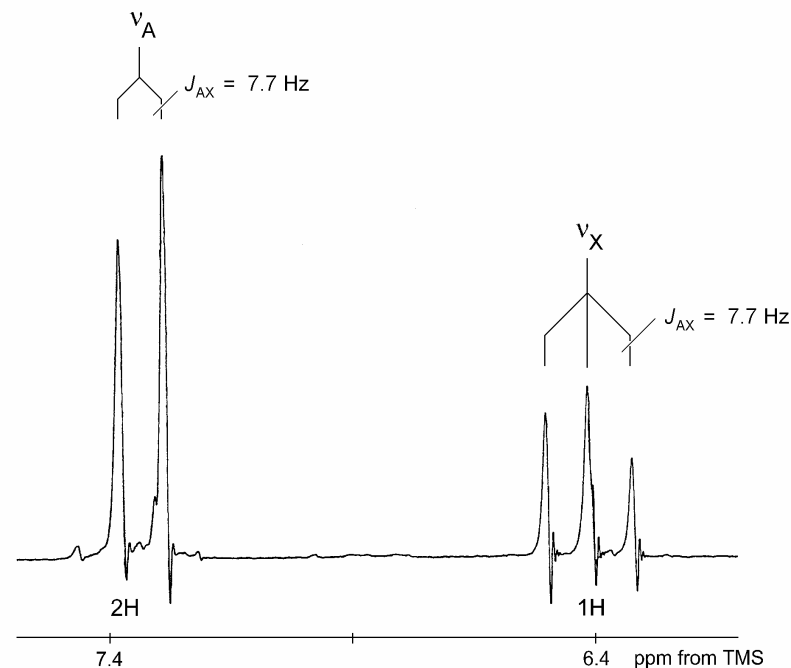
Chemical Shifts

$$\delta_A = 80 \text{ Hz} / 60 \text{ MHz} = 1.33 \text{ ppm}$$

$$\delta_M = 220 \text{ Hz} / 60 \text{ MHz} = 3.67 \text{ ppm}$$

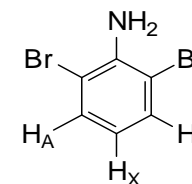
$$\delta_X = 320 \text{ Hz} / 60 \text{ MHz} = 5.33 \text{ ppm}$$

Problem 330 3 Spin System A<sub>2</sub>X



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<sub>2</sub>X 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

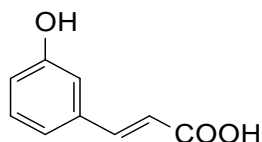
The spectrum is obtained after D<sub>2</sub>O exchange so the carboxylic acid and phenolic protons will not be present and the spectrum only contains the aromatic and vinylic protons.

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  $\delta$  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  $\delta$  6.4 is clearly one of the vinylic protons and it is coupled to the other vinylic proton at  $\delta$  7.6. The coupling constant is 16 Hz and this characteristic of vinylic protons which are *trans* to each other.

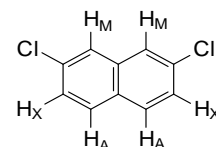
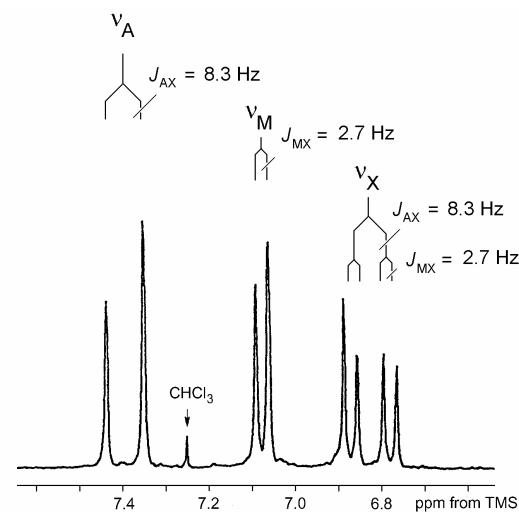
The correct answer is compound **3**.



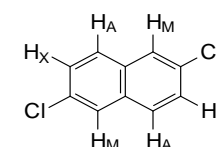
### Problem 332

All of the protons in the <sup>1</sup>H spectrum 1,5-dichloronaphthalene 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  $\delta$  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