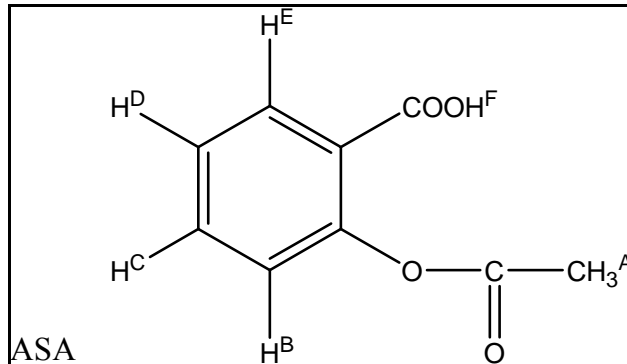


**T4b Practice problems** (Refer to page C36 in the online manual)

1. Predict the  $^1\text{H}$  nmr spectrum of acetylsalicylic acid (ASA) by:

a) predicting the shift of the protons using the tables in appendix A (yellow pages) of the manual. Show your work for any calculated values.

b) predicting the multiplicity assuming aromatic coupling of  $^4J_{\text{HH}}$  can be resolved.



$\text{H}^{\text{X}}$	shift, $\delta$ (ppm)	multiplicity	coupling constants (Hz)
A	<b>2.4</b> <i>p. A6: <math>\text{CH}_3\text{-CO-O-Ar}</math></i>	<i>s</i>	-
B	<b>7.23</b> <i>p. A4: <math>7.27 - 0.2</math> (<i>o</i>-OCOR) + <math>0.16</math> (<i>m</i>-COOH)</i>	<i>dd</i>	$^3J_{\text{BC}} = 8$ $^4J_{\text{BD}} = 2$
C	<b>7.62</b> <i>p. A4: <math>7.27 + 0.1</math> (<i>m</i>OCOR) + <math>0.25</math> (<i>p</i>--COOH)</i>	<i>td</i>	$^3J_{\text{CB and CD}} = 8$ $^4J_{\text{CE}} = 2$
D	<b>7.23</b> <i>p. A4: <math>7.27 - 0.2</math> (<i>p</i>-OCOR) + <math>0.16</math> (<i>m</i>-COOH)</i>	<i>td</i>	$^3J_{\text{DC and DE}} = 8$ $^4J_{\text{DB}} = 2$
E	<b>8.17</b> <i>p. A4: <math>7.27 + 0.80</math> (<i>o</i>-COOH) + <math>0.1</math> (<i>m</i>-OCOR)</i>	<i>dd</i>	$^3J_{\text{ED}} = 8$ $^4J_{\text{EC}} = 2$
F	<b>9-13</b> <i>p. A5: RCOOH</i> <b>OR 10-12</b> <i>p. A3: RCOOH</i>	<i>s</i>	-

- Print a completed copy of the above table and bring it with you to the lab. It will likely mean you are able to leave early.
- Watch the Royal Society of Chemistry video on proton NMR instrumentation at <http://www.youtube.com/watch?v=uNM801B9Y84&feature=relmfu>, or follow the link from the tutorial website.

