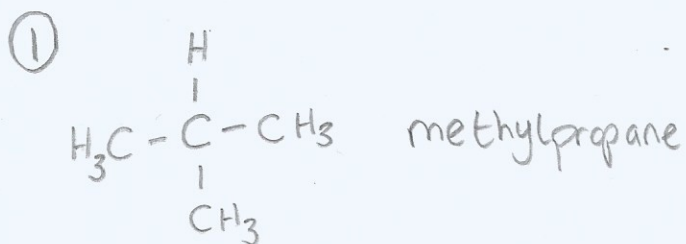


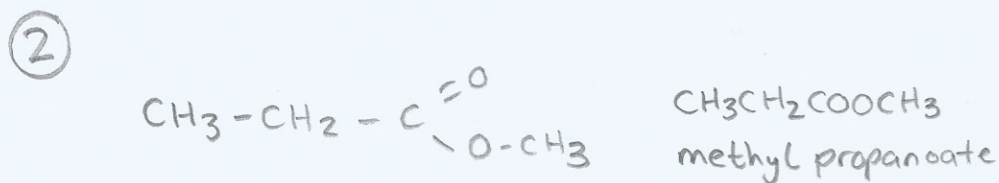
# 'H NMR Answers



Nmr - peak @ 1.5 has 1 hydrogen so CH  
peak @ 1 has 9 hydrogens so  $3 \times \text{CH}_3$

% mass gives empirical formula of  $\text{C}_2\text{H}_5$ , coupled with  
+ mass spec molecular ion peak of 58 gives  $\text{C}_4\text{H}_{10}$ .

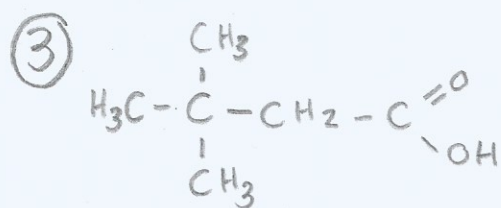
IR : confirms C-H bonds.



Nmr - peak @ 4.1ish has 3 hydrogens and using chemical shifts is  $\text{COOCH}_3$   
peak @ 2.5ish has 2 hydrogens and using chemical shifts is  $\text{CH}_2\text{-COO}$   
peak @ 1.1ish has 3 hydrogens and using chemical shifts is  $\text{CH}_3\text{-CH}_2$

% mass gives empirical formula  $\text{C}_2\text{H}_4\text{O}$ , coupled with  
+ mass spec molecular ion peak of 88 gives  $\text{C}_4\text{H}_8\text{O}_2$ .

IR : around  $1750\text{cm}^{-1}$  confirms carbonyl



3,3-dimethylbutanoic acid.

Nmr - peak @ 12 has 1 hydrogen and chemical shift suggests COOH.

peak @ 2.5 has 2 hydrogens and chemical shifts suggest CH<sub>2</sub>-COOH

peak @ 1 has 9 hydrogens so (CH<sub>3</sub>)<sub>3</sub>

% mass gives empirical formula of C<sub>3</sub>H<sub>6</sub>O, coupled with  
mass spec<sup>+</sup> molecular ion peak of 116 gives C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>.

IR : around 1700-1725 cm<sup>-1</sup> suggests carbonyl (ketone or COOH?)  
broad peak at 2450-3150 suggests hydroxyl group (alcohol or COOH?)