Department of Chemistry

# Mole Calculations Answers

1a. $M_r$ of $CH_3OH$ = 12.0 + (3 x 1.01) + 16.0 + 1.01 = 32.0 g mol$^{-1}$

1b. Moles $CH_3OH$ = mass / $M_r$ = 5.0 / 32.0 = 0.16 mol
(Answer to 2 significant figures as mass given to 2 significant figures.)

2. $M_r$ of $CO_2$ = 12.0 + (16.0 x 2) = 44.0 g mol$^{-1}$
Mass of $CO_2$ = $M_r$ x moles = 44.0 g x 0.50 g mol$^{-1}$ = 22 g

3a. $M_r$ = mass / moles = 54 / 3 = 18 g mol$^{-1}$

3b. It could be water ($H_2O$)

4. $M_r$ of $CuCO_3$ = 108 g mol$^{-1}$
Moles of $CuCO_3$ = mass / $M_r$ = 9.0 / 124 = 0.073 mol
$M_r$ of $CuCO_3$ = 63.5 + 12.0 + (3 x 16.0) = 123.5 = 124 (to 3 sf)

5a. Mass of $Br_2$ = density x volume = 3.1 x 2.0 = 6.2 g

5b. $M_r$ of $Br_2$ = 160 g mol$^{-1}$
Moles of $Br_2$ = mass / $M_r$ = 6.2 / 160 = 0.039 mol

6. Mass of Fe = moles x $M_r$ = 0.25 x 55.8 = 14 g

7. Moles of cyclohexane = mass / $M_r$ = 3.0 / 84.1 = 0.036 mol
$M_r$ of cyclohexane ($C_6H_{12}$) = (6 x 12.0) + (12 x 1.01) = 84.1

8. Mass benzene = moles x $M_r$ = 4.00 x 78.1 = 312 g
$M_r$ of benzene ($C_6H_6$) = (6 x 12.0) + (6 x 1.01) = 78.1

9a. Moles of tetrabutylammonium bromide ($Bu_4N^+ Br^-$) = mass / $M_r$
= 1.0 / 322 = 0.0031 mol
$M_r$ of $Bu_4N^+ Br^-$ ($C_{16}H_{36}BrN$) = (16 x 12.0) + (36 x 1.01) + 79.9 + 14.0 = 322

9b. 0.0031 moles of $Br_2$

9c. Mass $Br_2$ = moles x $M_r$ = 0.0031 x 160 = 0.496 = 0.50 g
Volume = mass / density = 0.50 / 3.10 = 0.16 $cm^{-3}$

10a. Electrophilic substitution.
Sulfuric acid protonates nitric acid to form, on loss of water, the nitronium ion (a strong electrophile):

$$HO–NO_2 + H^+ \longrightarrow H_2O^+–NO_2 \longrightarrow H_2O + {}^+NO_2$$

10b. Moles added:
methyl benzoate ($C_8H_8O_2$)
$M_r$ = (8 x 12.0) + (8 x 1.01) + (2 x 16.0) = 136
Moles = mass / $M_r$ = (6.0 / 136) = 0.044 mol

nitric acid ($HNO_3$)
Mass = volume x density = 4.0 x 1.51 = 6.0 g
$M_r$ = 1.01 + 14.0 + (3 x 16.0) = 63.0
Moles = mass / $M_r$ = (6.0 / 63.0) = 0.095 mol

sulfuric acid ($H_2SO_4$)
Mass = volume x density = 16.0 x 1.83 = 29.3 g
$M_r$ = (2 x 1.01) + 32.0 + (4 x 16.0) = 98.0
Moles = mass / $M_r$ = (29.3 / 98.0) = 0.299 mol

Methyl benzoate is the limiting reagent as there are only 0.044 mol of it

10c. 0.044 moles of product could be made

10d. Theoretical mass of product = $M_r$ x moles = 181 x 0.044 = 7.96 = 8.0 g
methyl 3-nitrobenzoate ($C_8H_7NO_4$)
$M_r$ = (8 x 12.0) + (7 x 1.01) + 14.0 + (4 x 16.0) = 181

10e. Methyl 3-nitrobenzoate

10f. Methyl 2-nitrobenzoate and methyl 4-nitrobenzoate

11a. An esterification reaction
A catalyst is a substance that increases the rate of a chemical reaction without being consumed in the reaction

11b. Mass of ethyl ethanoate formed = volume x density = 6.40 x 0.90 = 5.76 g

$CH_3CO_2H + CH_3CH_2OH \longrightarrow CH_3CO_2CH_2CH_3 + H_2O$

The carboxylic acid is ethanoic acid ($CH_3CO_2H$)
$M_r$ = (12.0 x 2) + (4.0 x 1.01) + (2 x 16.0) = 60.0
Moles = mass / $M_r$ = (6.0 / 60.0) = 0.10 mol

The alcohol is ethanol ($CH_3CH_2OH$)
$M_r$ = (12.0 x 2) + (6.0 x 1.01) + 16.0 = 46.1
Moles = mass / $M_r$ = (6.0 / 46.1) = 0.13 mol

Ethanoic acid is the limiting reagent as there are only 0.10 mol of it

Theoretical mass of ester = $M_r$ x moles = 88.1 x 0.10 = 8.81 g
$M_r$ of ester ($CH_3CO_2CH_2CH_3$) = (4 x 12.0) + (8 x 1.01) + (2 x 16.0) = 88.1

% yield = actual yield / theoretical yield x 100
% yield = 5.76 g / 8.81 g x 100 = 65.4% (to 1 dp, 3 sf) = 65% (rounding up)

11c. Atom economy = $M_r$ of desired product / combined $M_r$ of all reactants x 100
88.1 / (60.0 + 46.1) x 100 = 83.0% (to 1 dp, 3 sf) = 83% (rounding up)
(Note: 17% will be wasted)

11d. Conversion of $RCO_2H$ into $RCO_2R$ leads to a change in the wavenumber of the intense C=O stretching vibration, from around 1710 $cm^{-1}$ for $RCO_2H$ to around 1740 $cm^{-1}$ for $RCO_2R$. The peak intensities at 1710 $cm^{-1}$ and 1740 $cm^{-1}$ can be used to monitor the progress of the reaction.