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# THE CALCULATION OF STOICHIOMETRIC MIXTURES

by

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Summary

Simple formulae have been deduced from which the percentage volume and weight of the vapour of an organic compound in a stoichiometric mixture in air may be obtained. Values for some common organic compounds have been plotted.

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## Introduction

During work on the combustion of flammable gas and vapour mixtures, it is frequently necessary to know the amount of gas or vapour required to give a stoichiometric mixture with air. The calculation of the amount required, by volume or by weight, can be simplified by the application of the formulae deduced below.

## Volume Calculation

Complete combustion of the compound whose vapour has the molecular formula $C_C H_H O_O$ can be represented by equation 1.

$$C_C H_H O_O + \left(C + \frac{H}{4} - \frac{O}{2}\right) O_2 \longrightarrow C\ CO_2 + \frac{H}{2} H_2O \qquad \ldots\ldots (1)$$

If V volumes of $C_C H_H O_O$ are oxidised to carbon dioxide and water by combustion in air containing 20.8% oxygen, the volume of air equivalent to V volumes of $C_C H_H O_O$ is $\frac{100}{20.8}\left(C + \frac{H}{4} - \frac{O}{2}\right) V$

If the total volume of $C_C H_H O_O$ and air is 100,

$$V + \frac{100}{20.8}\left(C + \frac{H}{4} - \frac{O}{2}\right)V = 100 \qquad \ldots\ldots (2)$$

$$\therefore \quad V = \frac{100}{1 + 1.20\ (4C + H - 2O)} \qquad \ldots\ldots (3)$$

where V is the percentage by volume of $C_C H_H O_O$ in a stoichiometric mixture. If $4C + H - 2O$ is replaced by $x$, equation 3 becomes

$$V = \frac{100}{1 + 1.2x}\ \% \qquad \ldots\ldots (4)$$

and if V is plotted against $x$, a direct relationship is obtained from which the composition of the stoichiometric mixture by volume can be obtained for any given compound after deriving the appropriate value of $x$ by inspection of the molecular formula of the compound in question.

The function $V = \frac{100}{1 + 1.2x}\ \%$ is represented in figure 1, and the percentage volumes of members of various homologous series required for stoichiometric combustion are shown in figure 2.

## Weight Calculation

If V is the percentage by volume of the vapour in the stoichiometric mixture, then it follows that the percentage by weight will be given by

$$W = \frac{\rho V}{\rho V + q(100 - V)} \times 100\% \qquad \ldots\ldots (5)$$

where $W$ = percent weight of compound
$\rho$ = relative density of vapour of compound
$q$ = relative density of air

Replacing $\rho$ by $\frac{M}{2}$ where M is the molecular weight, and V by $\frac{100}{1 + 1.2x}$, and $q$ by 14.4,

$$W = \frac{\frac{M \times 100 \times 100}{1 + 1.2x}}{\frac{100M}{1 + 1.2x} + 2880 - \frac{2880}{1 + 1.2x}} \qquad \ldots\ldots (6)$$

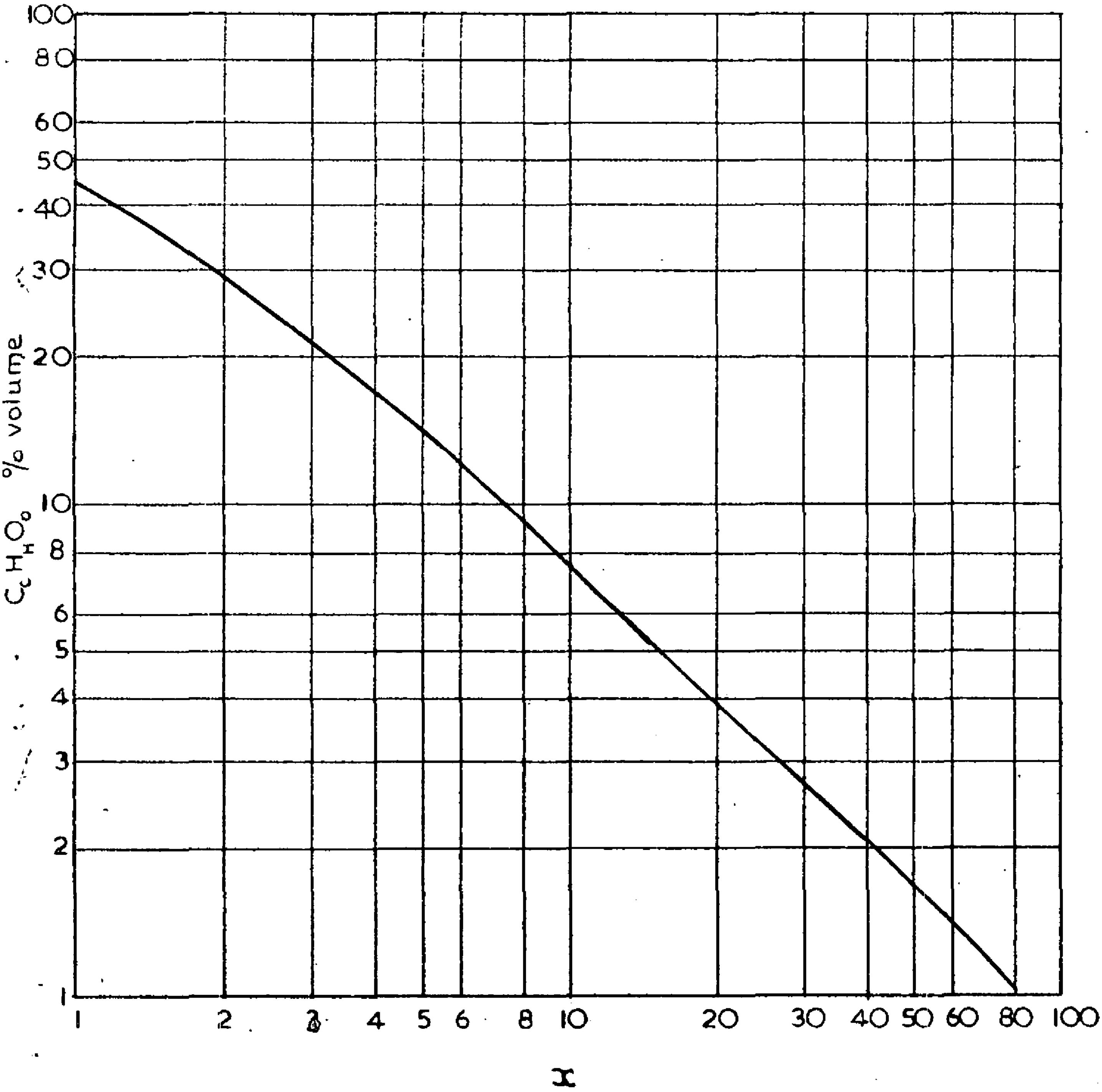
$$\text{or} \qquad W = \frac{100}{1 + 34.6\frac{x}{M}} \qquad \ldots\ldots (7)$$

The value of $\frac{x}{M}$ for various homologues is shown in table 1.

Table 1

| Series | Formula | $\frac{x}{M}$ |
|---|---|---|
| paraffins | $C_nH_{2n+2}$ | $\frac{3n+1}{7n+1}$ |
| olefines | $C_nH_{2n}$ | $\frac{3}{7}$ |
| acetylenes | $C_nH_{2n-2}$ | $\frac{3n-1}{7n-1}$ |
| alcohols | $C_nH_{2n+1}OH$ | $\frac{3n}{7n+9}$ |
| aldehydes | $C_nH_{2n+1}CHO$ | $\frac{3n+2}{7n+15}$ |
| fatty acids | $C_nH_{2n+1}COOH$ | $\frac{3n+1}{7n+23}$ |
| ethers | $C_nH_{2n+2}O$ | $\frac{3n}{7n+9}$ |
| ketones | $C_nH_{2n+2}CO$ | $\frac{3n+2}{7n+15}$ |
| alkylbenzenes | $C_6H_{6-n}(CH_3)_n$ | $\frac{3n+15}{7n+39}$ |

The percentage weight for members 1-14 of each series (and 0 where applicable) and 0-7 for the alkylbenzenes is shown in figure 3.




$x = 4C + H - 2O$

C = number of carbon atoms
H = number of hydrogen atoms
O = number of oxygen atoms

} in the molecule

FIG. 1. STOICHIOMETRIC MIXTURES

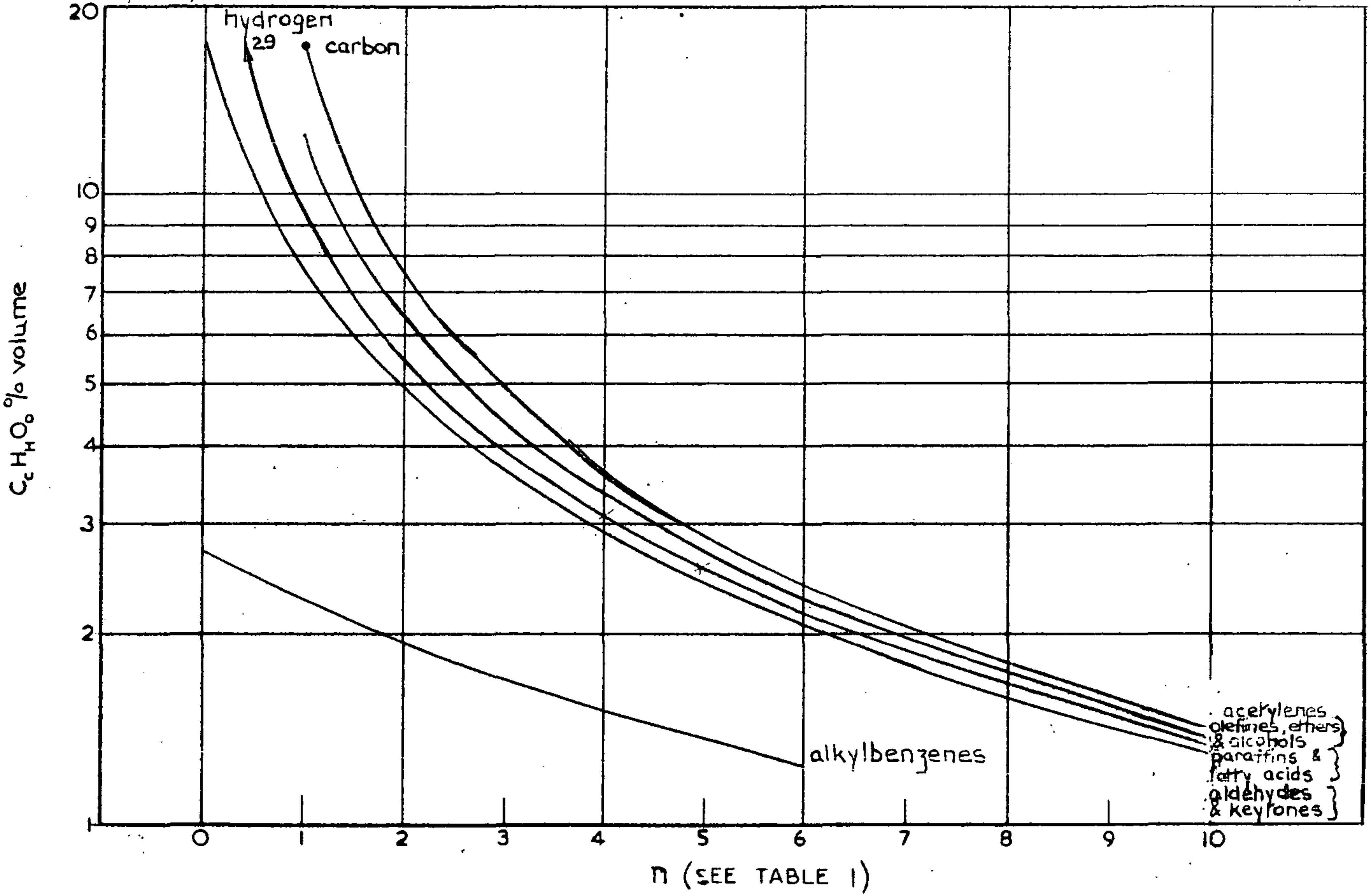



FIG. 2. STOICHIOMETRIC MIXTURES OF HOMOLOGOUS SERIES by volume

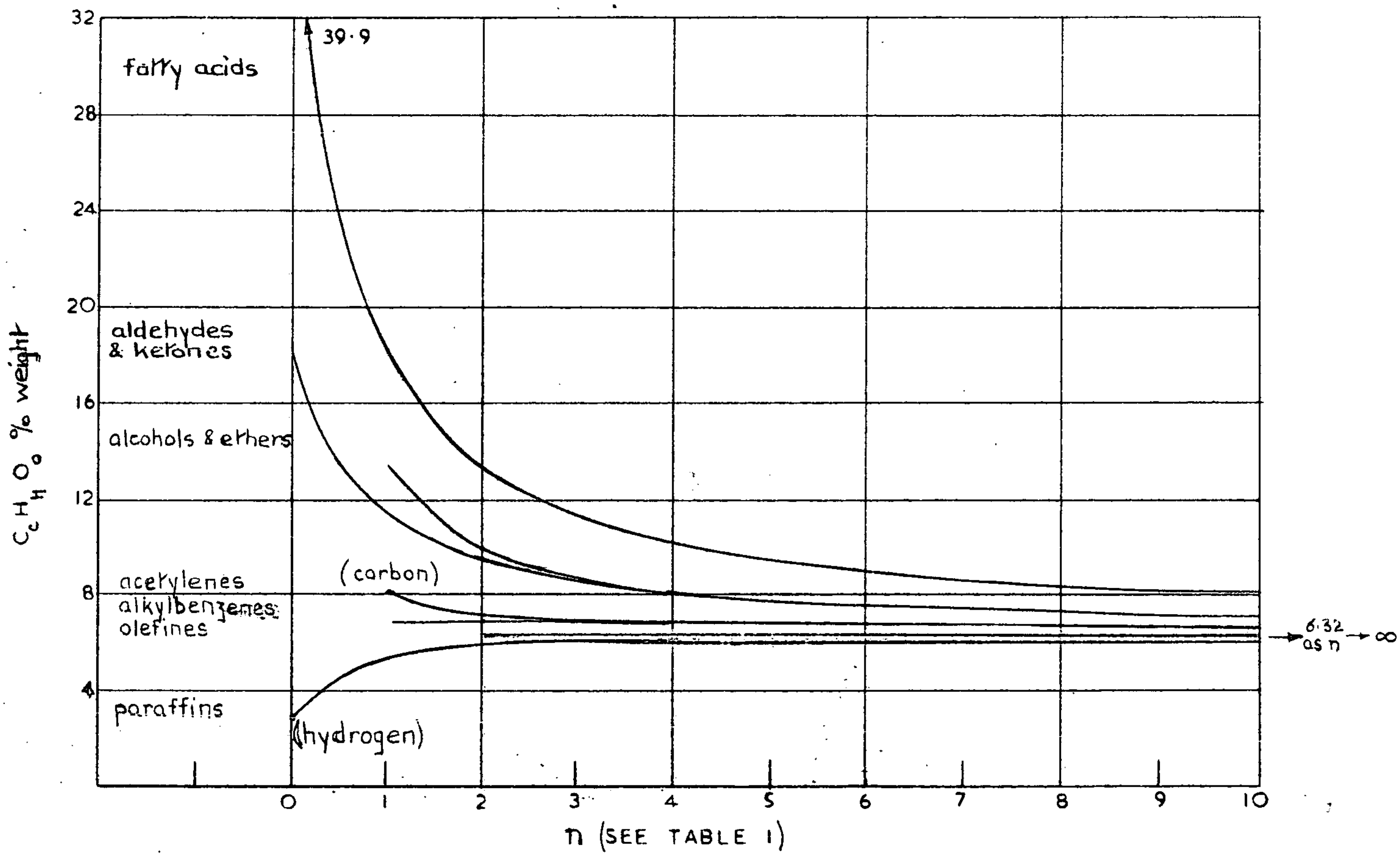



FIG. 3. STOICHIOMETRIC MIXTURES OF HOMOLOGOUS SERIES by weight