



# Psychrometric charts for organic vapours 1. Ketones in air

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Received 9 February 2004; accepted 30 March 2004

## Abstract

Psychrometric charts for five different condensing ketone vapours in air at 100 kPa are presented. The charts are based upon semi-theoretical equations and make use of published physical property data and correlations. The behaviour of the vapour phase is characterised by the virial equation of state truncated at the third term. The solubility of gas in the liquid ketones is also considered. The charts are constructed with the dry bulb temperature and absolute humidity scales as the orthogonal axes. Curves of constant adiabatic saturation temperature, constant relative humidity, constant gas specific volume and constant enthalpy deviation are plotted on the charts.  
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*Keywords:* Psychrometric charts; Ketones; Virial equation; Humidity; Acetone

## 1. Introduction

Psychrometric charts are a way in which physical property data may be presented diagrammatically for systems in which one component of a gaseous mixture may condense. While accurate charts are readily available for the conventional water–air system, only recently have charts been prepared for other important systems [1]. Ketones are an important class of chemical finding application as solvents and widely used as starting and intermediate ingredients in the production of a range of materials including resins, plastics and lacquers. As the vapour pressures of these ketones can be relatively high even at ambient temperatures significant levels of ketone vapours can exist in air when they are being used. For example, even at just 21 °C as much as 0.70 kg of propanone (the commercially-important solvent acetone) vapour can exist per 1 kg of dry air.

The author described the theory behind the construction of psychrometric charts [1–3]. In this paper this method will be applied to construct a series of psychrometric

charts for five ketone vapours in air. The five ketones are propanone, 2-butanone, 3-methyl-2-butanone, 3-pentanone and 2-hexanone. All charts are prepared for a total system pressure of 100 kPa.

## 2. Gas phase behaviour and saturation

At even relatively low pressures the gas mixture of ketone vapour and air will not behave ideally. From the many different methods by which the non-ideal behaviour of gas may be characterized, the virial equation of state is used. This method is chosen because it is relatively simple to apply and because considerable data is available for the required parameters for each of the systems studied. The virial equation of state truncated at the third term is:

$$\frac{P_T \hat{V}}{RT} = 1 + \frac{B_m}{\hat{V}} + \frac{C_m}{\hat{V}^2} \quad (1)$$

where,  $P_T$  is the total pressure,  $\hat{V}$  is the molar volume of the gas mixture,  $R$  is the gas constant,  $T$  is the absolute temperature, and  $B_m$  and  $C_m$  are the second and third virial coefficients of the gas, respectively.

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### Nomenclature

$B$	second virial coefficient	$T_{\text{datum}}$	enthalpy datum temperature
$c$	correlation coefficient	$T_r$	reduced temperature
$C$	third virial coefficient	$\widehat{V}_C$	critical volume
$C_P$	ideal gas heat capacity	$\widehat{V}_{V_c}$	liquid molar volume
$f$	enhancement factor	$x$	mole fraction
$g_1, g_2$	functions defined in Eqs. (A.14) and (A.15)	$Z_C$	critical compressibility factor
$\hat{h}$	real gas specific enthalpy	<i>Greek letters</i>	
$\hat{h}_{\text{dev}}$	enthalpy deviation	$\phi$	relative humidity
$\hat{h}_f$	condensed phase enthalpy	$\kappa$	isothermal compressibility
$\hat{h}'_0$	enthalpy correction	$\lambda$	latent heat of vaporization
$k_H$	Henry's law constant	$\omega$	acentric factor
$MW$	molecular weight	<i>Subscripts</i>	
$P_C$	critical pressure	$G$	non-condensing gas component, i.e., air
$P_V$	vapour pressure	$m$	mixture
$P_T$	total pressure	$S$	saturation condition
$R$	Universal gas constant	$V$	condensing vapour component, i.e., ketone vapour
$T$	absolute temperature		
$T_{\text{ad}}$	adiabatic saturation temperature		
$T_C$	critical temperature		

In the development of the equations which follows we shall assume that there are only two components in our system. The vapour component that readily condenses (i.e., the ketone) will be denoted  $V$ , and the gas component (i.e., the air) will be denoted  $G$ .

If  $x_G$  is the mole fraction of the non-condensing component (in this case nitrogen) and  $x_V$  is the mole fraction of the condensing component (i.e., the alcohol) then for a binary system it may be shown that:

$$B_m = x_G^2 B_{GG} + 2x_G x_V B_{GV} + x_V^2 B_{VV} \quad (2)$$

$$C_m = x_G^3 C_{GGG} + 3x_G^2 x_V C_{GGV} + 3x_G x_V^2 C_{GVV} + x_V^3 C_{VVV} \quad (3)$$

Here  $B_{ii}$  is the second virial coefficient of pure component  $i$ ,  $B_{GV}$  is the second virial interaction (or cross) coefficient for the binary system,  $C_{iii}$  is the third virial coefficient of pure component  $i$ , and,  $C_{GGV}$  and  $C_{GVV}$  are the third virial interaction parameters. The virial coefficients are all functions of temperature alone, and are either known or may be estimated for most binary systems.

A gas is saturated with a vapour when the partial pressure of the vapour is equal to its vapour pressure at the particular temperature. For an ideal system we could write an expression relating the mole fraction of the condensing vapour component at saturation,  $V$ , to its vapour pressure:

$$x_{V_s} = \frac{P_V}{P_T} \quad (4)$$

and

$$x_{G_s} = \frac{P_T - P_V}{P_T} \quad (5)$$

where,  $x_{V_s}$  and  $x_{G_s}$  are the mole fractions of components  $V$  and  $G$  respectively at saturation, and  $P_V$  is the vapour pressure of component  $V$ . However, since the system is not ideal Hyland and Wexler [4] proposed the use of an enhancement factor. Eq. (4) becomes,

$$x_{V_s} = \frac{f P_V}{P_T} \quad (6)$$

A similar expression may be written for the non-condensing gas component  $G$ :

$$x_{G_s} = \frac{P_T - f P_V}{P_T} \quad (7)$$

The enhancement factor accounts for the effects of the dissolved gases and pressure on the properties of the condensed phase, and the effect of intermolecular forces on the properties of the moisture itself. Typically the value for the enhance factor does not exceed 1.05 for any given system [1]. The enhancement factor may be written in terms of the virial coefficients and other properties of the system [4]:

$$\begin{aligned} \ln f = & \left[ \frac{(1 + \kappa P_V)(P_T - P_V) - \frac{1}{2}\kappa(P_T^2 - P_V^2)}{RT} \right] \widehat{V}_{V_c} \\ & + \ln(1 - k_H x_{G_s} P_T) + \frac{x_{G_s}^2 P_T}{RT} B_{GG} - \frac{2x_{G_s}^2 P_T}{RT} B_{GV} \\ & - \left[ \frac{P_T - P_V - x_{G_s}^2 P_T}{RT} \right] B_{GG} \\ & - \frac{2x_{G_s}^3 (2 - 3x_{G_s}) P_T^2}{(RT)^2} B_{GG} B_{GV} \\ & - \frac{x_{G_s}^2 (1 - 3x_{G_s})(1 - x_{G_s}) P_T^2}{(RT)^2} B_{GG} B_{VV} \end{aligned}$$

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