VAPOUR PRESSURE EQUATIONS FOR 2-PHENOXYETHANOL AND ACETYL- PHENOXYETHANOL

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abstract: The parameters of Wrede-Auguste and Antoine's equations have been calculated for 2-phenoxyethanol ($C_8H_{10}O_2$) and acetyl-2-phenoxyethanol ($C_{10}H_{12}O_3$), used as fixatives per parfumes in organic synthesis, as bactericides and topical antiseptics.

Introduction

The present paper attempts to establish the Wrede-Auguste and Antoine's parameters of vapour pressure equation based on experimental measurements and using the author's calculation program [1].

The vapour pressures at various temperatures were measured in a statically – based principle installation, previously described [2] in the range 350 – 425 K.

The measurement were carried out at different temperatures, following 5-6 successive operation of freezing with liquid nitrogen and degassing with a vacuum aggregate to 10^{-4} mmHg pressure. The manometer readings were performed by a cathetometer with an accuracy of ± 0.01 mmHg.

Experimental

The measurements were carried out using a static installation based on the isotensioscope method. It [2] consist of four principle parts: the equilibrium still, the measurement and compensation system, the vacuum system (10^{-6} torr) and the degassing and sample introducing device.

The samples were degassed into the equilibrium cell following 6 – 7 successive cycles of freezing with liquid nitrogen and pumping to high vacuum. The vacuum system contains a McLead gauge which gives as the opportunity to measure high vacuum of the installation.

The equilibrium cell was introduced in an oil bath and thermostating temperature was measured with an accuracy of 0.5 K.

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Since desired temperature was performed the vapour pressure of the substances was compensated and measured by an external mercury manometer. The manometer readings were performed by a cathetometer with an accuracy of ± 0.01 mmHg.

The performance of the installation was already analyzed [2].

Results and discussions

These substances are used as fixatives for perfumes in organic synthesis, and they have bactericide as well as antiseptic effect. So is very important to know their vapour pressure at low temperature, the closest to standard ones.

Substances were synthesized products of the first grade of purity checked by GC. The evidence of the purity (better than 99%) is illustrated in Table 1. The physical properties of used substances and LD_{50} are also shown in Table 1.

Table 1. Physical properties of substances.

Substance	M (g/mol)	T_m (K)	T_b (K)	V_m (m^3/kmol)	n_D^{20}	ρ_{20} (Kg/m^3)	Antoine's parameters *P*(kPa) and T(K)			LD_{50} (g/Kg)
							A	B	C	
2-phenoxyethanol	138.16	287.15 [3]	518.05 [3]	0.1254 [3]	1.534 [4] 1.535 this work	1.194 [4] 1.110 this work	6.69552 [4]	2033.96 [4]	-84.761 [4]	1.26
							(in the 351-519K)			
acetyl-2-phenoxyethanol	183.16	376.45 [3]	523.35 [5]	0.1623 [3]	1.5232 [5] 1.5280 this work	1.057 [5] 1.063 this work	8.1156 [4]	3422.32 [4]	27.331 [4]	0.93
							(in the 355-533K)			

In Table 1 LD_{50} means medium lethal dose equal with quantity of chemicals that is estimated to be fatal to 50% of organism tested.

The experimental saturation vapour pressure obtained for substances in the range 350-430K are presented in Table 2.

Figs. 1 and 2 represent P (mmHg) $= f\,[t(^{o}C)]$ and $\lg T = f(1/T)$.

Using the calculation program earlier presented [1] the Wrede-Auguste and Antoine's parameters were calculated and presented in Table 3.

Table 2. Saturated vapour pressure versus temperature (°C)

2-phenoxyethanol		acetyl-2-phenoxyethanol	
t (°C)	P (mmHg)	t (°C)	P (mmHg)
84.5	0.7	92.0	1.8
90.1	1.1	95.3	2.2
95.0	1.7	100.1	2.7
101.2	2.8	105.6	3.6
105.6	3.4	110.4	4.5
109.9	4.8	114.9	5.6
115.2	7.0	120.1	7.1
119.0	8.7	125.6	9.1
125.7	12.7	131.2	11.6
131.0	16.0	135.8	14.0
135.3	19.4	141.2	17.5
		146.5	21.6
		151.0	25.7

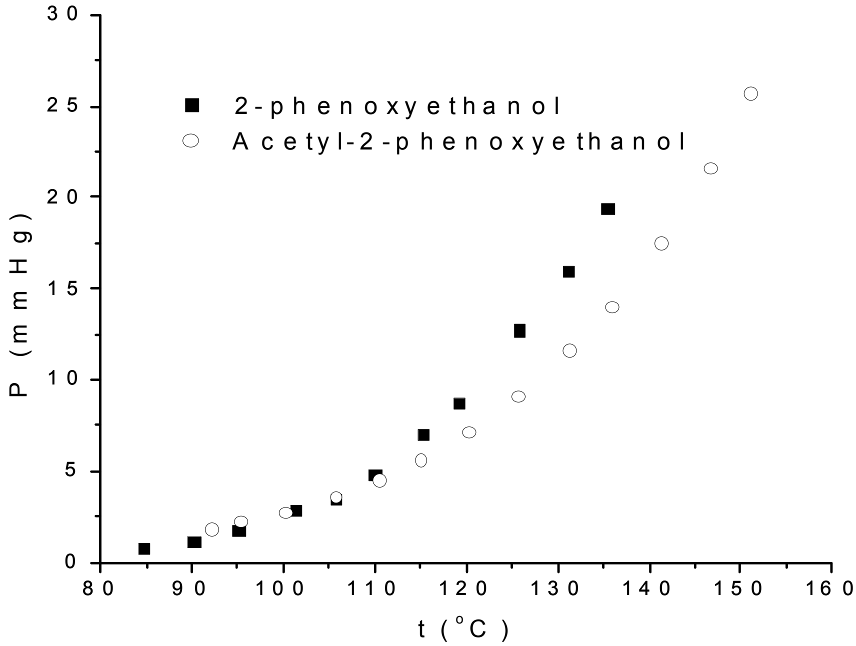

Fig. 1. *Vapour pressure versus temperature for substances.*

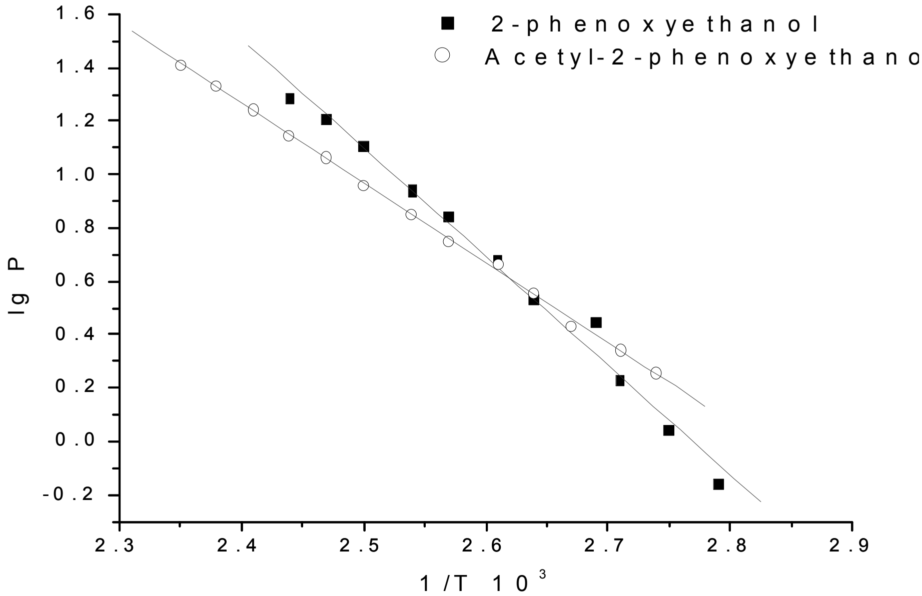

Fig. 2. lg $P = f(1/T)$

Table 3. Wrede-Auguste and Antoine's parameters.

Substance	Wrede-Auguste equation		Antoine equation		
	A	B	A	B	C
2-phenoxyethanol	9.15482	3213.36	3.9709	386.947	8.435
acetyl-2-phenoxyethanol	7.59933	2633.30	9.56265	3918.188	327.7

In Table 4 are listed the experimental and calculated vapour pressure as well as the values of relative and average standard deviation δ (P) calculated with the equations:

$$\delta(P) = \frac{P_{\exp} - P_{\text{calc}}}{P_{\exp}} \cdot 100 \text{ and } \delta(P) = \left[\frac{\Sigma\left(P_{\exp} - P_{\text{calc}}\right)^2}{N - f} \right]^{\frac{1}{2}}$$

were N is the number of experimental points and f is the number of constant in correlation equations.

Table 4. Experimental vapour pressure, calculated vapour pressure and relative and average standard deviation.

t (°C)	$\frac{1}{T}\cdot 10^3$	P_{exp} (mmHg)	lg *P*	$P_{calc.}$ W–A	$P_{calc.}$ A	Deviation $\delta(P)=\frac{P_{exp}-P_{calc}}{P_{exp}}\cdot 100$ W–A	$\delta(P)=\frac{P_{exp}-P_{calc}}{P_{exp}}\cdot 100$ A	$\delta(P)=\left[\frac{\Sigma(P_{exp}-P_{calc})^2}{N-f}\right]^{\frac{1}{2}}$ W–A	$\delta(P)=\left[\frac{\Sigma(P_{exp}-P_{calc})^2}{N-f}\right]^{\frac{1}{2}}$ A
2–phenoxyethanol									
84.5	2.79	0.7	–0.156	1.48	0.65	–	7.10		
90.1	2.75	1.1	0.041	2.03	1.12	–	–1.80		
95.0	2.71	1.7	0.230	2.60	1.73	–	–1.76		
101.2	2.69	2.8	0.447	3.72	2.82	–	–0.71		
105.6	2.64	3.4	0.531	4.08	3.39	–	0.29		
109.9	2.61	4.8	0.681	4.82	4.83	–	–0.62	0.404	0.0418
115.2	2.57	7.0	0.845	7.59	7.07	0.625	–0.42		
119.0	2.54	8.7	0.939	9.00	8.76	0.689	–0.68		
125.7	2.5	12.7	1.104	12.54	12.76	0.472	–0.47		
131.0	2.47	16.0	1.204	15.99	15.99	0.062	0.06		
135.3	2.44	19.4	1.287	19.40	19.36	0.206	0.20		
						$\bar{\delta}$ =0.410	$\bar{\delta}$ =–0.591		
acetyl–2–phenoxyethanol									
92.0	2.74	1.8	0.255	2.42	1.86	–4.44	–3.33		
95.3	2.71	2.2	0.342	2.73	2.20	0.00	0.00		
100.1	2.67	2.7	0.431	2.90	2.79	–3.33	–0.33		
105.6	2.64	3.6	0.556	3.71	3.65	–1.38	–1.38		
110.4	2.61	4.5	0.663	4.44	4.57	0.65	0.65		
114.9	2.57	5.6	0.748	5.32	5.62	10.35	–0.35		
120.1	2.54	7.1	0.851	8.14	7.11	–14.64	–0.14	1.6	0.0447
125.6	2.50	9.1	0.959	10.37	9.06	–13.95	0.43		
131.2	2.47	11.6	1.064	12.44	11.53	–7.24	0.60		
135.8	2.44	14.0	1.146	14.90	13.99	–6.40	0.07		
141.2	2.41	17.5	1.243	17.91	17.47	–2.34	0.34		
146.5	2.38	21.6	1.332	21.48	21.60	0.09	–0.04		
151.0	2.35	25.7	1.411	25.70	25.82	0.00	–0.07		
						$\bar{\delta}$ =11.09	$\bar{\delta}$ =–0.22		

From Table 4 we can identify the best vapour pressure correlation equation for substances which is Antoine's so far. For 2-phenoxyethanol, in the temperature range of 350-425 K average standard deviation is 0.0418 while for acetyl-2-phenoxyethanol is 0.0447.

The Wrede-Auguste correlates the saturation vapour pressure of 2- phenoxyethanol in the range 288-308 with a relative deviation of 0.41 but doesn't correlate the acetyl-2-phenoxyethanol data. The error is too high.

The experimental saturation vapour pressures are as we expected, small in that temperature range. This is the reason for their cosmetical and antiseptic use.

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