Saturated vapour pressures of 2-(2-hydroxy-5-methyl-phenyl)benzotriazole and some derivatives of 2,4-dihydroxybenzophenone

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Some data about the saturated vapour pressures of seven organic compounds, *i.e.* 2-(2-hydroxy-5-methylphenyl)benzotriazole and six derivatives of 2,4-dihydroxybenzophenone, measured by the effusion method in the temperature interval 100—180 °C are presented in this paper. The experimental values were used for calculating the constants in the Antoine equation.

В работе приводятся данные по давлениям насыщенных паров семи органических соединений: 2-(2-гидрокси-5-метилфенил)бензотриазола и шести производных 2,4-дигидроксибензофенона в интервале температур 100—180 °С, измеренных методом эффузии. На основе экспериментальных данных рассчитаны константы для уравнения Антуана.

2-(2-Hydroxy-5-methylphenyl)benzotriazole (*I*), 2-hydroxy-4-ethyloxybenzophenone (*II*), 2-hydroxy-4-n-butyloxybenzophenone (*III*), 2-hydroxy-4-n-butyloxy-5-*tert*-butylbenzophenone (*IV*), 2-hydroxy-4-(2-ethylhexyloxy)benzophenone (*V*), 2-hydroxy-4-n-octyloxybenzophenone (*VI*), and 2-hydroxy-4-n-dodecyloxybenzophenone (*VII*) are compounds belonging into the group of additives for polymer substances which are called UV-absorbers. The application of these substances at the thermal treatment of polymers brings about a decrease in their content in polymer by evaporation, which causes an impaired stabilization and loss of expensive additive. For this reason, we determined the saturated vapour pressures of these compounds and the results are summarized in this paper.

The pressures of saturated vapour were measured by the effusion method the basic theory of which is discussed in papers [1—4]. The principle of this method is based on the measurement of effusion rate of substance vapour getting out of

a vessel through a very small circular hole with exactly known diameter. In contrast to some authors [5—9] who determined the mass loss of the investigated substance during evaporation *in vacuo* by weighing the vessel containing the sample before and after experiment, we determined the mass loss from the change in length of a spring balance according to papers [3, 10—15]. This method makes possible to determine the pressure of saturated vapour of a given substance with greater accuracy. As a matter of fact, the weighing of effusion vessel with sample proceeds continuously and thus we can determine the mass loss in arbitrary moment from the start of experiment and repeat the measurement several times under equal conditions. This method also enables us to deprive the sample of possibly present volatile components before measurement.

Experimental

Chemicals and apparatus

All investigated compounds were synthesized in laboratory* and purified by crystallization except *V* which was dissolved in n-hexane, the insoluble residue was separated, and the solvent removed by vacuum distillation. The effusion of substance was measured with an apparatus which, in the main, corresponded to the apparatus described by *Sklyarenko et al.* [3]. The effusion vessel consisted of thin-walled glass, its mass being up to 500 mg. The quartz spring had 50 turns with internal diameter of 25 mm, the thickness of fibre of 0.300 mm, and the maximum working load 1 g. The dimension of effusion hole was measured with an Abbe comparator, the accuracy being 0.001 mm.

Results and discussion

The saturated vapour pressure was calculated from the following equation

$$\frac{P}{[J\ K^{-1}\ mol^{-1}]^{1/2}} = \frac{m}{s\ t}\left(\frac{T}{M}\right)^{1/2} \times 7.2261 \qquad (1)$$

The Clausing correction factor [4] was omitted in the calculation with respect to the thickness of the used cap and size of the effusion holes. The pressures of saturated vapour of individual compounds are listed in Table 1.

* The compounds were prepared in the department of rubber chemicals and additives for polymer substances of the Research Institute of Chemical Technology.
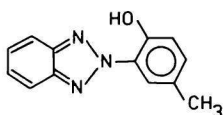
Table 1

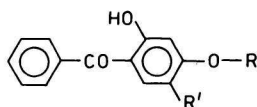Characteristics of the investigated compounds and their saturated vapour pressures

Compound	Formula $M/(g\ mol^{-1})$ M. p./°C	θ/°C	P/Pa
I	$C_{13}H_{11}N_3O$	131	37.48
	225.251	140	64.70
	131	145	85.79
		150	112.38
		155	145.51
		160	187.54
II	$C_{15}H_{14}O_3$	100	2.95
	242.276	120	14.45
	55.5	130	29.16
		140	55.16
		150	98.23
		160	168.65
III	$C_{17}H_{18}O_3$	120	7.51
	270.330	130	16.50
	56	140	32.80
		150	60.85
		160	109.07
		170	187.06
IV	$C_{21}H_{26}O_3$	130	3.81
	326.439	140	7.48
	89	150	14.00
		160	25.65
		170	44.01
		180	74.11
V	$C_{21}H_{26}O_3$	120	0.50
	326.439	140	2.33
	< -15	150	4.37
		160	8.51
		165	11.13
		170	15.51
VI	$C_{21}H_{26}O_3$	140	1.57
	326.439	150	2.95
	48	160	5.96
		170	11.15
		175	15.74
		180	21.10

Table 1 (Continued)

Compound	Formula $M/(\text{g mol}^{-1})$ M.p./°C	θ/°C	P/Pa
VII	$C_{25}H_{14}O_3$	140	0.14
	382.547	150	0.30
	49	160	0.61
		170	1.35
		175	1.93
		180	2.65

I   *II – VII*

The measured values of the saturated vapour pressures of *I* are confronted with the data published by *Schmitt* and *Hirt* [16] in Fig. 1. It results from this plot that the data presented in this paper are between the values calculated by means of the equation published by these authors for the liquid state and the values obtained by extension of the line describing the dependence of the pressures of saturated vapour on temperature for the solid substance.
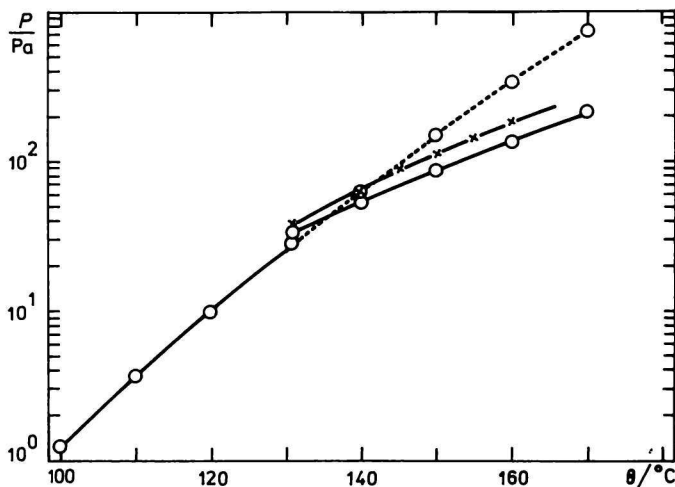

Fig. 1. Values of saturated vapour pressures of 2-(2-hydroxy-5-methylphenyl)benzotriazole obtained by us (x) and the values obtained by *Schmitt* and *Hirt* [16] (o).

Fig. 2 represents the variation of the pressure of saturated vapour with temperature for other six compounds, *i.e.* derivatives of 2,4-dihydroxybenzophenone. These relationships were expressed by the Antoine equation
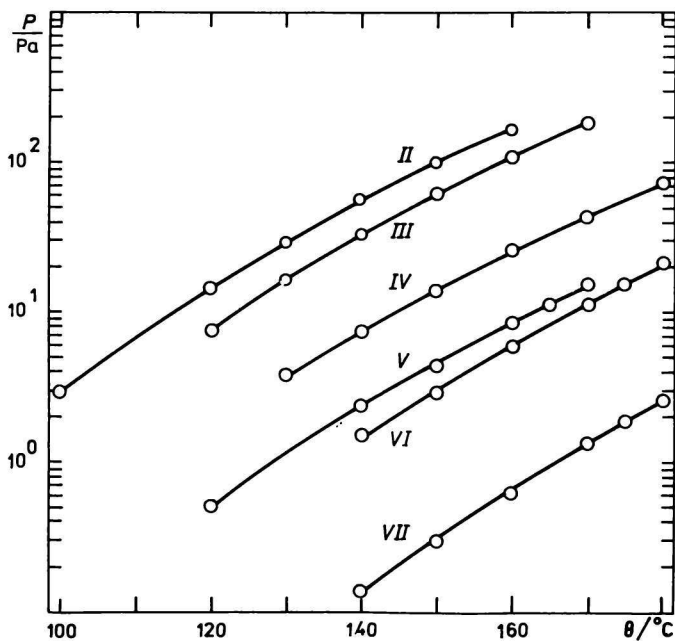

Fig. 2. Variation of saturated vapour pressure of individual investigated substances with temperature.

Table 2

Coefficients in the Antoine equation and the mean and maximum deviations of the measured values of saturated vapour pressure from the calculated values

Compound	Temperature interval $\Delta\theta/°C$	A	B	C	$\sum_i |P - \hat{P}|_i/n$ Pa	$(P - \hat{P})_{max}$ Pa
I	131—160	7.86644	1463.96	101.72	0.16	0.32
II	100—160	8.04958	1508.62	99.09	0.11	−0.23
III	120—170	8.45611	1695.42	104.16	0.14	0.30
IV	130—180	9.01511	2341.95	147.76	0.09	−0.21
V	120—170	9.04650	2460.88	143.10	0.11	0.33
VI	140—180	9.46294	2550.56	133.58	0.14	0.37
VII	140—180	9.74248	2987.49	140.99	0.03	0.07

$$\log \hat{P}/\text{Pa} = A - \frac{B}{C + \theta/°C} \tag{2}$$

the coefficients of which were determined by minimization of the function

$$\text{M}(A, B, C) = \sum_{i=1}^{n} (P - \hat{P})_i^2 \tag{3}$$

by means of the Gauss—Newton method. The values of coefficients in the Antoine equation are given for individual compounds in Table 2 together with the mean and maximum deviation of the measured values of saturated vapour pressures from the calculated values.

The measured data in Table 1 and plots in Fig. 2 show that the pressure of saturated vapour of substance decreases with increasing length of the chain. These results confirm the known fact that a branched chain (compound *IV* and *V*) is less favourable when compared with normal chain (compound *VI*) from the view-point of nonvolatility and the nearer to the ring (compound *IV*) is the branching, the higher is the saturated vapour pressure.

Symbols

P	saturated vapour pressure (measured)	Pa
$\hat{P}$	saturated vapour pressure (calculated)	Pa
A, B, C	coefficients in the Antoine equation	
M	molecular mass	kg mol^{-1}
T	absolute temperature	K
m	mass of effused substance	kg
s	area of effusion hole	m^2
θ	temperature	°C
t	time of effusion	s

Indices

i	i-th measurement
n	number of measurements

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