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N.S. Zefirov on His 70th Anniversary

Polynomial Dependence for the Calculation of Vaporization Enthalpies of Organophosphorus Compounds

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Abstract—Enthalpies of vaporization of organic phosphorus compounds are related to the normal-pressure boiling points through a polynomial dependence. Each class of organophosphorus compounds is characterized by its own specific parameters of the general dependence. The polynomial dependences may be used for the calculation of vaporization enthalpies of organophosphorus compounds with different modes of phosphorus coordination.

Most of the known experimental enthalpies of vaporization of organic three- and four-coordinate phosphorus compounds were determined by two methods. The first of these is based on the Clapeyron–Clausius equation [1]:

$$\ln p = -\Delta H_{\text{vap}}/RT + C, \quad (1)$$

where p is the vapor pressure; ΔH_{vap} is the enthalpy of vaporization (kJ/mol), R is the universal gas constant, T is the absolute temperature, and C is the integration constant.

The second method is based on the Solomonov equation [2, 3]:

$$\Delta H_{\text{vap}} = \Delta H_{\text{dis}} + a + bMR_{\text{D}}, \quad (2)$$

where ΔH_{dis} is the enthalpy of dissolution of a substance (kJ/mol), and MR_{D} is its molecular refraction.

However, both these procedures for experimental determination of $\Delta H_{\text{vap}}^{\circ}$ of organophosphorus compounds are not free from a number of disadvantages which could appreciably restrict the scope of their application in practice. For example, the use of the Clapeyron–Clausius equation is limited due to high boiling points of organic phosphorus compounds which therefore tend to decompose on heating. Determination of the enthalpies of dissolution of organophosphorus compounds in inert organic solvents,

which are necessary for the calculation of vaporization enthalpies by the Solomonov equation, is not always possible due to insufficient stability of these compounds to oxidation on exposure to atmospheric oxygen and to hydrolysis in the presence of traces of water. Taking into account the above stated, theoretical methods for the calculation of vaporization enthalpies of organophosphorus compounds become more important. In particular, the additivity scheme involving group contributions [4] can be used for this purpose:

$$Y = m_1 X_1 + m_2 X_2 + \dots + m_i X_i. \quad (3)$$

Here, m_i is the number of similar fragments in a molecule, and X_i is an increment characterizing the group contribution of an i th fragment. However, the calculation of standard enthalpies of vaporization of organic phosphorus compounds according to the additivity scheme may be difficult, for there are very limited published data on the contributions of phosphorus-containing groups to $\Delta H_{\text{vap}}^{\circ}$. The relevant data have been reported in a few articles [5, 6]. Moreover, the possibility for calculating contributions of phosphorus-containing groups to the enthalpy of vaporization of organophosphorus compounds is limited due to shortage of experimental data and, in some cases, large errors in experimental determination.

In the recent time, attempts were made [7–10] to calculate enthalpies of vaporization of three-coordinate

phosphorus compounds using linear relations between $\Delta H_{\text{vap}}^{\circ}$ and boiling points, which are expressed by the Troughton equation (4) [11] and Wadso equation (5) [1] proposed previously for estimation of enthalpies of vaporization of unassociated and weakly associated organic liquids:

$$\Delta H_{\text{vap}} = 4.184K(0.00176t_b + 0.253), \quad (4)$$

where K is the Troughton constant equal to 21–22 for most unassociated organic liquids [12], and t_b is the normal-pressure boiling point ($^{\circ}\text{C}$); and

$$\Delta H_{\text{vap}} = 4.184[5.0 + 0.041(T_b - 273)], \quad (5)$$

where T_b is the boiling point (K) at 760 mm.

According to [7–10], a good agreement was found between the experimental enthalpies of vaporization and those calculated by Eqs. (4) and (5) for a large number of P(III) derivatives. In addition, enthalpies of vaporization were calculated for some organophosphorus compounds for which no experimental data were available. In continuation of our previously initiated studies, we calculated the enthalpies of vaporization of about 50 P(III) compounds belonging to 7 different classes with a view to compare the results with the experimental data. As in [7–10], we used the same equations (4) and (5).

Table 1 contains relative (percent) deviations of the $\Delta H_{\text{vap}}^{\circ}$ values calculated by Eqs. (4) and (5) from the corresponding experimental data. If a calculated $\Delta H_{\text{vap}}^{\circ}$ value was greater than experimental, the deviation was assumed to be positive, otherwise it was assumed to be negative [24]. As follows from the data in Table 1, in most cases no satisfactory agreement between the calculated and experimental $\Delta H_{\text{vap}}^{\circ}$ values is observed. For example, the accuracy in the calculation of the enthalpy of vaporization of triphenylphosphine (**18**) by both Eq. (4) and Eq. (5) is so unsatisfactory that the calculated $\Delta H_{\text{vap}}^{\circ}$ values are quite inconsistent with the five known experimental values obtained by different authors (Table 1).

In the series of five-membered cyclic phosphorochloridites **39–42**, Eq. (4) gives no ΔH_{vap} values coinciding with the corresponding experimental enthalpies of vaporization. The percent deviations of the ΔH_{vap} values calculated by Eq. (4) from the experimental data range from 10.0 to 15.5% (Table 1). An analogous pattern is observed for ΔH_{vap} of compounds **39–42**, calculated by Eq. (5).

Lapteva and co-workers [7–10] used four different correlation equations, including Eqs. (4) and (5), and obtained several calculated enthalpies of vaporization for each organophosphorus compound, which often strongly differed from each other. The reasons for such discrepancy in the calculated $\Delta H_{\text{vap}}^{\circ}$ values were not analyzed, and the obtained values were simply averaged. Figures 1 and 2 illustrate the corresponding deviations of the ΔH_{vap} values calculated by the Troughton equation from those found experimentally for two classes of organophosphorus compounds. It is seen that mutual arrangement of plots 1 and 2 in Figs. 1 and 2 (and hence the character of agreement or disagreement between the calculated and experimental ΔH_{vap} values with rise in the enthalpies of vaporization or boiling points) is specific for each particular class of phosphorus(III) compounds. In the series of tertiary alkylphosphines (Fig. 1), Eq. (4) gives overestimated values of the enthalpy of vaporization up to the crossing point of plots 1 and 2 (at about 200°C), while after that point the calculated ΔH_{vap} values are underestimated. The corresponding crossing point for acyclic alkyl phosphites (Fig. 2) is located at about 115°C , and the enthalpies of vaporization of all compounds of this series, calculated by Eq. (4), are underestimated (Table 1). A complete agreement between the calculated and experimental enthalpies of vaporization of P(III) derivatives is observed only in the region of crossing of plots 1 and 2. In particular, the enthalpy of vaporization of trimethyl phosphite (**26**, t_b 111°C), calculated by Eq. (4), approaches the corresponding experimental value ($\Delta H_{\text{vap}} = 41.3$ and 40.6 kJ/mol, respectively; Fig. 2).

Analogous pattern was observed for the experimental and calculated [by Eqs. (4) and (5)] enthalpies of vaporization of organic compounds; therefore, we decided [25] that the linear character of the $\Delta H_{\text{vap}}-t_b$ relation is doubtful. We then found that enthalpies of vaporization of organic compounds are related to their normal-pressure boiling points through the following polynomial dependence:

$$\Delta H_{\text{vap}} = a + b_1 t_b + b_2 t_b^2, \quad (6)$$

where a , b_1 , and b_2 are empirical coefficients which are specific for each class of organic compounds, and t_b is the boiling point ($^{\circ}\text{C}$) at 760 mm.

It is easy to conclude that, as with other organic compounds, the reason of the clear disagreement between the calculated and experimental enthalpies of vaporization of P(III) derivatives (Table 1) is the linear

Table 1. Experimental and calculated enthalpies of vaporization, group increments of phosphorus-containing fragments, boiling points, and percent deviations of the calculated values from experimental (298 K)



Comp. no.	Compound	bp (t_b), °C	Group increment, kJ/mol	$\Delta H_{\text{vap}}^{\circ}$, kJ/mol		Deviation, ^a %		
				experiment	calculated by Eq. (3)	Eq. (4)	Eq. (5)	Eq. (6)
Alkylphosphines								
			P-(C)(H) ₂					
1	MePH ₂	-14	15.84 ^b	22.2 [13]	22.3	-5.3	-16.6	-
2	<i>cyclo</i> -C ₆ H ₁₁ PH ₂	146	23.30	52.5 [14]	45.2	-10.6	-12.4	-
3	H ₂ P(CH ₂) ₂ PH ₂	113	15.96 ^b	38.1 [8]	38.1	9.2	5.8	-
4	H ₂ P(CH ₂) ₃ PH ₂	143	14.67	40.3 [8]	42.8	15.3	12.8	-
Dialkylphosphines								
			P-(C) ₂ (H)					
5	Me ₂ PH	21	13.48 ^b	26.2 [15]	26.5	1.9	-6.4	-
6	MeEtPH	55	15.18	31.0 [8]	29.6	3.9	-2.1	-
7	MePrPH	78	14.61 ^b	35.2 [8]	34.4	2.1	-2.6	-
8	MeBuPH	113	8.94	34.3 [8]	39.2	21.3	17.5	-
9	 PH	37	13.30 ^b	29.2 [16]	29.7	0.3	-6.6	-
10	 PH	105	15.62	37.8 [8]	36.0	6.6	3.0	-
Trialkylphosphines								
			P-(C) ₃					
11	Me ₃ P	39	9.92 ^b	29.0 [17]	29.6	2.1	-4.8	-0.1
12	Me ₂ EtP	71	10.52 ^b	32.7 [18]	32.7	6.4	1.2	-3.1
13	(Et) ₃ P	128	11.13 ^b	39.5 [18]	38.9	11.5	8.6	0.4
14	Pr ₃ P	188	4.02	46.7 [18]	53.2	15.1	13.9	12.4
15	Bu ₃ P	241	-3.39	53.6 [18]	67.5	16.3	16.2	26.1
16	(<i>i</i> -Bu) ₃ P	210 ^c	-1.46	49.5 [18]	61.5	15.8	15.0	17.8
			P-(C _d) ₃					
17	Vin ₃ P	117	10.97 ^b	37.2 [18]	37.2	13.6	10.2	1.6
			P-(C _v) ₃					
18	Ph ₃ P	384	-18.77	71.1 [18]		20.3	22.1	
			4.23	94.1 [20]		-9.1	-7.8	
			6.33	96.2 [1]		-11.1	-9.8	
			23.33 ^b	113.2 [21]	113.2	-24.5	-23.3	-
			28.43	118.3 [22]		-27.7	-26.6	
Alkyldichlorophosphines								
			P-(C)(Cl) ₂					
19	EtPCl ₂	112	25.44 ^b	34.9 [18]	34.7	18.7	15.0	0.3
20	PrPCl ₂	135	24.97 ^b	39.2 [18]	39.5	15.2	12.4	-0.1
21	BuPCl ₂	160	23.10	42.1 [18]	44.2	16.9	14.9	4.5
22	AmPCl ₂	184	18.43	42.2 [18]	49.0	25.8	24.4	15.8
23	C ₆ H ₁₃ PCl ₂	208	16.77	45.3 [18]	53.8	25.8	24.9	19.3
24	C ₇ H ₁₅ PCl ₂	229	14.60	47.9 [18]	58.5	26.1	25.7	22.7
25	C ₈ H ₁₇ PCl ₂	247	13.23	51.3 [18]	63.3	23.4	23.4	22.9

Table 1. (Contd.)

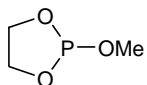
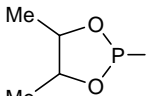
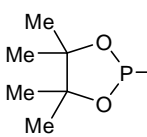
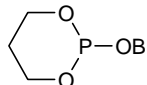
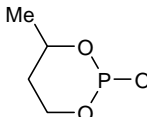
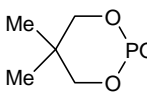
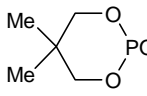
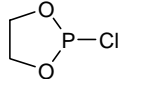
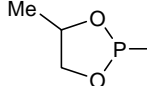
Comp. no.	Compound	bp (<i>t_b</i>), °C	Group increment, kJ/mol	$\Delta H_{\text{vap}}^{\circ}$, kJ/mol		Deviation, ^a %		
				experiment	calculated by Eq. (3)	Eq. (4)	Eq. (5)	Eq. (6)
Trialkyl phosphites								
			$3[\text{O}-(\text{C})(\text{P})] + \text{P}-(\text{O})_3$					
26	(MeO) ₃ P	111	21.52	40.6 [14]	40.8	1.7	-1.6	0.2
			18.62	37.7 [17]		9.5	6.0	7.9
27	(EtO) ₃ P	159	24.63	53.0 [14]	50.1	-7.5	-9.1	-0.6
			13.43	41.8 [1]		17.3	15.3	26.0
28	(PrO) ₃ P	200 ^c	3.32	46.0 [17]	64.4	21.1	20.1	40.0
29	(<i>i</i> -PrO) ₃ P	191	26.51	61.4 [14]	56.7	-11.7	-12.6	0.5
			11.11	46.0 [1]		17.9	16.7	34.1
30	(BuO) ₃ P	250 ^c	23.51	80.5 [14]	78.7	-20.8	-20.7	-0.1
Five-membered cyclic trialkyl phosphites								
31		140 ^c	22.60	41.6 [14]	40.8	10.5	8.0	-
32		170 ^c	23.66	50.1 [14]	48.2	1.5	0.0	-
33		175 ^c	19.27	51.4 [14]	53.9	0.5	-0.9	-
Six-membered cyclic trialkyl phosphites								
34		200 ^c	21.70 ^b	58.1 [14]	58.2	-4.1	-4.9	0.1
35		170 ^c	22.56	51.6 [14]	50.8	-1.5	-2.9	-5.8
36		168 ^c	18.83	48.2 [14]	51.1	4.8	3.2	0.1
37		180 ^c	20.33	52.8 [14]	54.2	-0.7	-1.9	-3.8
Dialkyl phosphorochloridites								
38	(EtO) ₂ P-Cl	150 ^c	$2[\text{O}-(\text{C})(\text{P})] + \text{P}-(\text{O})_2(\text{Cl})$ 29.59	48.5 [14]	46.7	-1.9	-3.8	-
Five-membered cyclic dialkyl phosphorochloridites								
39		145 ^c	27.86 ^b	40.5 [14]	40.4	15.5	13.1	0.0
40		150 ^c	26.59	41.4 [14]	42.6	14.9	12.7	-0.4

Table 1. (Contd.)

Comp. no.	Compound	bp (t_b), °C	Group increment, kJ/mol	$\Delta H_{\text{vap}}^{\circ}$, kJ/mol		Deviation, ^a %		
				experiment	calculated by Eq. (3)	Eq. (4)	Eq. (5)	Eq. (6)
41		161 ^c	27.91 ^b	44.9 [14]	44.8	10.0	8.1	-4.4
42		190 ^c	25.32	48.0 [14]	50.5	12.6	11.5	0.0
Six-membered cyclic dialkyl phosphorodichloridites								
43		170	27.09	44.5 [14]	45.2	14.2	12.5	-
44		175	27.52 ^b	47.1 [14]	47.4	9.6	8.2	-
45		175	23.99	47.0 [14]	50.8	9.9	8.4	-
Alkyl phosphorodichloridites								
			O-(C)P + P-(O)(Cl) ₂					
46	MeOPCl ₂	95	30.94 ^b	37.3 [14]	37.3	3.7	-0.2	-0.1
47	EtOPCl ₂	117	30.94 ^b	40.4 [23]	40.4	4.6	1.5	-2.7
48	PrOPCl ₂	143	30.97 ^b	45.2 [14]	45.2	2.8	0.6	0.0
49	BuOPCl ₂	154	29.90	48.9 [23]	50.0	-1.4	-3.2	-0.2

^a Percent deviation of the enthalpies of vaporization calculated by Eqs. (4)–(6) from the corresponding experimental values.

^b The data were used to calculate group increments to the enthalpy of vaporization.

^c Boiling points of high-boiling compounds were recalculated to the standard conditions according to [19] with an accuracy of $\pm 10^{\circ}\text{C}$.

character of the $\Delta H_{\text{vap}}-t_b$ dependence in Eqs. (4) and (5). While further studying $\Delta H_{\text{vap}}-t_b$ relations for three- and four-coordinate phosphorus compounds, we have found that, as in the general case, the relation between the enthalpies of vaporization and boiling points of organophosphorus compounds is polynomial. Figure 3 shows some $\Delta H_{\text{vap}}-t_b$ dependences plotted

for particular classes of organic phosphorus compounds. Each class is characterized by specific values of the coefficients in Eq. (6). In contrast to [7–10], there is no common $\Delta H_{\text{vap}}-t_b$ dependence covering all classes of organophosphorus compounds. Table 2 contains the parameters of Eq. (6), calculated for particular classes of three- and four-coordinate phosphorus com-

Table 2. Parameters of Eq. (6) for three- and four-coordinate phosphorus compounds

Compound series	a	b_1	b_2	R	S_0	n
Trialkylphosphines	27.4	0.02	0.0006	0.99992	0.20	5
Alkyldichlorophosphines	18.3	0.12	0.0002	0.99953	0.27	7
Acyclic trialkyl phosphites	19.9	0.14	0.0004	0.99977	0.32	5
Six-membered cyclic phosphites	161.0	-1.5	0.005	0.99984	0.09	4
Five-membered cyclic phosphorochloridites	31.5	-0.02	0.0005	0.99998	0.02	4
Alkyl phosphorodichloridites	59.5	-0.5	0.003	0.99996	0.06	4
Dialkyl phosphonates	13.0	0.11	0.0003	0.99991	0.31	10

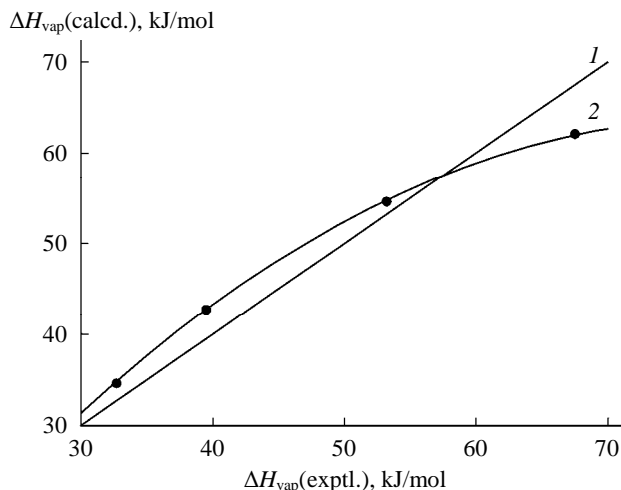


Fig. 1. Plots of (1) $\Delta H_{\text{vap}}(\text{exptl.})$ versus $\Delta H_{\text{vap}}(\text{exptl.})$ (bisector) and (2) ΔH_{vap} calculated by Eq. 4 versus $\Delta H_{\text{vap}}(\text{exptl.})$ for trialkylphosphines.

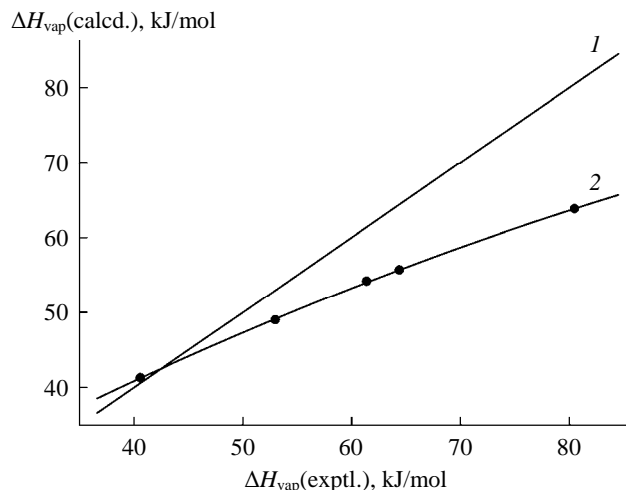


Fig. 2. Plots of (1) $\Delta H_{\text{vap}}(\text{exptl.})$ versus $\Delta H_{\text{vap}}(\text{exptl.})$ (bisector) and (2) ΔH_{vap} calculated by Eq. 4 versus $\Delta H_{\text{vap}}(\text{exptl.})$ for acyclic trialkyl phosphites.

pounds. Obviously, analogous polynomial relations may be deduced for other classes of organophosphorus compounds. Fairly high correlation coefficients and small standard deviations found for the dependences given in Table 2 give us grounds to use Eq. (6) for the calculation of enthalpies of vaporization of organophosphorus compounds from their boiling points. Unfortunately, the set of available experimental data for specific classes of organophosphorus compounds is now insufficient to calculate the corresponding parameters in Eq. (6).

It is seen (Table 1) that in most cases the enthalpies of vaporization of organophosphorus compounds, calculated by polynomial Eq. (6), are characterized by

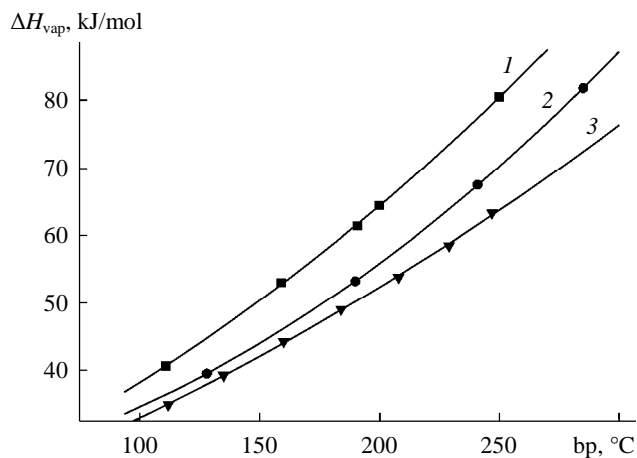


Fig. 3. Plots of the enthalpies of vaporization calculated by Eq. (6) versus boiling points for (1) acyclic trialkyl phosphites, (2) trialkylphosphines, and (3) alkyldichlorophosphines.

minimal percent deviations from the experimental values, as compared to those calculated according to linear relations (4) and (5). As noted in [5, 6], the method used for experimental determination of enthalpies of vaporization of organophosphorus compounds may strongly affect the accuracy of the results, and the accuracy may be estimated with the aid of the contributions of phosphorus-containing groups to $\Delta H_{\text{vap}}^{\circ}$. It is known that analysis of group contributions to enthalpy parameters of organic compounds could favor refinement and more correct treatment of the experimental data.

Table 1 contains the corresponding increments of phosphorus-containing groups to the enthalpy of vaporization of each compound. Fairly similar group increments to $\Delta H_{\text{vap}}^{\circ}$ were found within each series of a large number of P(III) derivatives, including cyclic alkyl phosphites 31–37, cyclic dialkyl phosphorochloridites 39–45, and alkyl phosphorodichloridites 46–49. In the series of acyclic trialkyl phosphites 26–30, the above stated applies to only those values which were calculated from the enthalpies of vaporization obtained by the Solomonov equation (2) [14]. The enthalpies of vaporization of trialkyl phosphites 26–29, calculated by the Clapeyron–Clausius equation (1) [1, 17], give P-increments appreciably different both from each other and from those calculated with the use of Eq. (2); furthermore, the difference increases as the boiling point rises.

Alkylphosphines whose enthalpies of vaporization were calculated only by Eq. (1) are characterized by considerable dispersion of the increments of phos-

Table 3. Group contributions X_i (kJ/mol) for the calculation of enthalpies of vaporization with the corresponding standard deviations S_0

Group	X_i	S_0	Group	X_i	S_0	Group	X_i	S_0
P-(C)(H) ₂	15.9	0.02	P-(C _d) ₃	11.0	–	3[O-(C)(P)] + P-(O) ₃	21.8	0.02
P-(C) ₂ (H)	13.8	0.17	P-(C _B) ₃	23.3	–	2[O-(C)(P)] + P-(O) ₂ (Cl)	27.8	0.05
P-(C) ₃	10.5	0.15	P-(C)(Cl) ₂	25.2	0.08	O-(C)(P) + P-(O)(Cl) ₂	31.0	0.01

Table 4. Calculated energies of vaporization (kJ/mol) and boiling points of organophosphorus compounds

Compound no.	Formula	Boiling point t_b , °C	$\Delta H_{\text{vap}}^{\circ}$	
			Eq. (3)	Eq. (6)
Trialkylphosphines				
50	Am ₃ P	285 ^a	81.8	82.8
51	(C ₆ H ₁₃) ₃ P	320 ^a	96.2	96.6
52	(C ₇ H ₁₅) ₃ P	355 ^a	110.5	112.0
Alkyldichlorophosphines				
53	MePCL ₂	82	31.6	30.0
54	C ₈ H ₁₇ PCL ₂	247	63.3	63.0
55	ClCH ₂ CH ₂ PCL ₂	170	45.8	46.0
Acyclic trialkyl phosphites				
56	(AmO) ₃ P	290 ^a	93.1	94.7
57	(C ₆ H ₁₃ O) ₃ P	330 ^a	107.4	110.2
58	(ClCH ₂ CH ₂ O) ₃ P	260 ^a	83.4	83.9
Alkyl phosphorodichloridites				
59	AmOPCL ₂	170 ^a	54.7	55.3
60	ClCH ₂ CH ₂ OPCL ₂	160 ^a	51.5	51.1
Dialkyl phosphonates				
61	(BuO) ₂ P(O)H	260 ^a	64.8	64.7
62	(AmO) ₂ P(O)H	290 ^a	74.3	73.7

^a The boiling points of high-boiling compounds were recalculated to the standard conditions according to [19] with an accuracy of $\pm 10^{\circ}\text{C}$.

phorus-containing groups for each class of compounds: primary alkylphosphines **1–4**, 14.67 to 23.30 kJ/mol; dialkylphosphines **5–10**, 8.94 to 15.62 kJ/mol; trialkylphosphines **11–16**, –3.39 to 11.13 kJ/mol; and alkyldichlorophosphines **19–25**, 13.23 to 25.44 kJ/mol. The group contributions to $\Delta H_{\text{vap}}^{\circ}$ decrease in absolute value as the boiling point rises within a homological series.

Thus increase in the boiling point within a series of three-coordinate phosphorus derivatives is accompanied by gradual reduction of the enthalpy of vaporization calculated by Eq. (1), as compared to the corresponding values calculated by Eq. (2), which is reflected in the contributions of phosphorus-containing groups to $\Delta H_{\text{vap}}^{\circ}$. Therefore, underestimated group increments to the enthalpies of vaporization of P(III) compounds, calculated by Eq. (1), were not taken into

account in the final calculation of averaged increments of phosphorus-containing groups (Table 3), and the enthalpies of vaporization of compounds **8**, **14–16**, **22–25**, and **28**, calculated just by the additivity scheme (3) (Table 1), should be regarded as the most reliable.

It should be noted that compounds **14–16** and **22–29** are characterized by large positive percent deviations of the $\Delta H_{\text{vap}}^{\circ}$ values calculated by polynomial Eq. (6) owing to underestimation of the corresponding experimental enthalpies of vaporization (Table 1). This is explained by the fact that the calculated enthalpies of vaporization exceed experimental $\Delta H_{\text{vap}}^{\circ}$ values obtained according to Eq. (1). The enthalpies of vaporization of compounds **14–16** and **22–29**, calculated by polynomial Eq. (6) and by the additivity scheme [Eq. (3)], are in a good agreement.

In support of the above stated, Table 4 contains ΔH_{vap} values of some three- and four-coordinate phosphorus derivatives, for which the corresponding experimental data are unavailable, calculated by the additivity scheme (Eq. (3)) using the data in Table 3 and [4] and by Eq. (6) (Table 2). A good agreement between the ΔH_{vap} values calculated by the two independent methods indicates reliability of the proposed approaches and their possible applicability for the calculation of enthalpies of vaporization of complex organophosphorus compounds with different modes of coordination of the phosphorus atom.

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