Thermochimica Acta 511 (2010) 107–111

Contents lists available at ScienceDirect

Thermochimica Acta

journal homepage: www.elsevier.com/locate/tca

Estimation of normal boiling points of trialkyl phosphates using retention indices by gas chromatography

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ARTICLE INFO

Article history:
Received 16 June 2010
Received in revised form 28 July 2010
Accepted 29 July 2010
Available online 6 August 2010

Keywords:
Trialkyl phosphates
Retention index
Normal boiling point
Topological indices
Regression analysis

ABSTRACT

Retention indices of several homologous trialkyl phosphates have been determined by gas chromatography on different polar stationary phases namely, Apiezon L, SE-30 and XE-60. Normal boiling points of these trialkyl phosphates have been evaluated and compared with available literature values. Topological indices such as *Xu* index, atom type index and steric effect index are derived for these phosphates and have been correlated with the normal boiling points using multiple regression analysis. The influences of alkyl chain length, relative position of alkyl branching and steric factors on retention index are investigated and also the effect of polarity of the stationary phase on retention indices is discussed.

1. Introduction

Trialkyl phosphates such as tri n-butyl phosphate (TBP) are important extractants in nuclear fuel reprocessing. PUREX (Plutonium Uranium Reduction EXtraction) is a well known aqueous reprocessing process where TBP [1–6] diluted in aliphatic hydrocarbons is employed to recover uranium and plutonium from irradiated nuclear fuel solution. Though TBP has been successfully employed for thermal reactor fuels over the past five decades, it has several shortcomings for fast reactor fuel reprocessing such as, third phase formation during the extraction of tetravalent metal ions, unacceptable aqueous solubility [7,8], hydrolytic and radiolytic degradation, and poor U (VI)/Th (IV) separation. Alternatives to TBP, such as tri-sec-butyl phosphate (TsBP), tri n-amyl phosphate (TAP), and triisoamyl phosphate (TiAP), which do not have the shortcomings of TBP but at the same time retain its merits have been developed and extensively studied in our laboratory. TsBP [9] and TiAP [10] have been found to be better candidates for THOREX (THORium uranium EXtraction) and PUREX process respectively. Trimethyl phosphate and triethyl phosphate find applications as fire retardant additives for rubber and plastic [11–14], plasticizers, insecticides, curing agents, stabilizers, anti-wear additives, lubricants etc.

Normal boiling point is an indispensable parameter for synthesis and is an important input for computing critical temperature, flash point, enthalpy of vaporization, etc. Normal boiling points have not been reported in the literature for several synthesized trialkyl phosphates, except triisobutyl phosphate. The direct measurement of boiling point for trialkyl phosphates is an extremely laborious, time-consuming and expensive process as it requires pure compounds. Also high molecular weight phosphates decompose prior to reaching their normal boiling points and necessitate measurements under reduced pressure and later corrections to ambient pressure leading to errors. In view of these shortcomings, development of reliable methods for estimating normal boiling points of these compounds is essential.

Gas chromatographic retention indices have been used in the present study for determining normal boiling point of trialkyl phosphates. This technique tolerates some impurities and enables estimation with high accuracy and precision. It is possible to obtain retention times of phosphates with widely ranging volatilities in a single temperature-programmed experimental run. Gas chromatographic retention mainly depends on the solute–stationary phase interactions resulting from the chemical, structural and electronic features of the compound of interest. The variation in the retention behaviour is due to the macrocosmic reflection of the molecular structures of the injected compounds and the stationary phase [15,16]. The retention index (RI) is usually determined by injecting the compound along with two n-alkanes whose retention times lie on either side under suitable temperature-programmed conditions

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doi:10.1016/j.tca.2010.07.032

and is given by the following equation [17,18]:

$$RI = 100N\left[\frac{t_{R(c)} - t_{R(z)}}{t_{R_{(z+n)}} - t_{R(z)}}\right] + 100_z \tag{1}$$

where N is the difference in carbon number between the two n-alkanes that elute before and after trialkyl phosphate, t_R is the retention time for the trialkyl phosphate and Z is the carbon number of the n-alkane eluting immediately prior to trialkyl phosphate. Molecules of trialkyl phosphates with higher electron density than corresponding number of carbon atoms of alkanes have higher retention.

A major part of the current research in the computational chemistry, graph theory and Quantitative Structure–Property Relationship (QSPR)/Quantitative Structure–Activity Relationship (QSAR) involves topological indices. QSPR/QSAR is important complementary tools in computational chemistry to represent explain and, most importantly, predict a variety of physicochemical [19–21], biomedical [22] and toxicological properties [23]. QSPR can give insight into the aspects of the molecular structure which in turn influences various properties and has been used extensively to explain separation mechanisms, physicochemical properties of solutes in thin-layer [24] and gas chromatographic [18,25] techniques.

Topological indices are numerical graph invariants that quantitatively parameterize molecular structure and can be directly derived from the structure of the molecule on the basis of graph theory without any experimental effort. They can easily be computed and used to predict many physicochemical properties. Nevertheless choice of an appropriate index is very essential for obtaining good correlation and hence an error free prediction. For example most of the conventional topological indices such as, Wiener index [26], Balaban index [27], Randic index [28], Hosoya index [29] and Schluze index [30] are found unsuccessful for compounds with multiple bonds and heteroatoms, since these indices do not take into account the contribution of each of the individual atom types or groups. Most of the physicochemical properties depend on individual atoms or groups, polarizability of the molecule, length of carbon backbone, shape and branching of the molecule and their contribution to the structural environment in the molecule. Structural parameters that represent the size and bulkiness of alkyl groups would be expected to largely contribute to physicochemical properties. Thus the atom type index "*AI*", representing structural features, *Xu* index "X_U" which reflects size and composition of the molecule and the steric effect index "SV_{ij}" which reflects bulkiness of the molecules have been derived for all the trialkyl phosphates studied and a correlation has been attempted to predict the normal boiling point [31–34] of these phosphates with these indices using a multiple linear regression analysis.

2. Experiments

2.1. Materials

A homologous series of n-alkanes ranging from n-heptane to n-heptacosane (TCI) which served as standards for determining retention index and trimethyl phosphate (TMP) (Merck), triethyl phosphate (TEP) (Merck), tri n-butyl phosphate (TBP) (Alfa aesar) were of commercial origin and used as received without any additional pre-treatment. Triisobutyl phosphate (TiBP), tri-sec-butyl phosphate (TsBP), triisoamyl phosphate (TiAP), tri-2-methyl butyl phosphate (T2MBP), tri-sec-amyl phosphate (TsAP) and trihexyl phosphate (THP) were synthesized according to the described method [35,36] by using corresponding alcohol with phosphoryl chloride and were further purified by distillation under reduced pressure after extensive washings with distilled water and characterization using FTIR spectrophotometry.

Table 1
Characteristics of chromatographic column, 10% of stationary phases are coated on chromosorb W (HP), 80/100 mesh.

Notation	Stationary phase	Polarity
Apiezon L	Higher molecular weight hydrocarbon grease	143
SE-30	Dimethylpolysiloxane	229
XE-60	Cyanoethyl methyl siloxane	1785

2.2. Methods

The retention times of trialkyl phosphate reference standards (TEP, TMP, TiBP and TBP) and unknowns (TsBP, TsAP, T2MBP, TiAP and TAP) were determined by injecting along with n-alkane standards by a temperature-programmed method on different polar stationary phases. A Shimadzu GC–9A gas chromatograph equipped with flame ionization detector (FID) incorporating a packed stainless steel column (3.2 mm OD × 4 m length) was used for retention time measurements. Splitless injector was used for sample introduction. Injection port and FID were set at 225 °C for vaporization and detection of eluted compounds. Argon was used as mobile phase at a constant flow rate of 50 mL/min. Hydrogen (50 mL/min) and air (500 mL/min) were fed into FID to aid the ignition of the eluted compounds. The characteristics of stationary phase used in the chromatographic column are summarized in Table 1. The temperature of the column oven was programmed from 100 °C to 225 °C at 1.5 °C/min, and held at 100 °C for 2 min and 225 °C for 25 min, as initial and final temperature, respectively. Data handling was carried out by ASHCO® software. Using the retention time of the phosphates and alkane standards the retention indices were evaluated.

2.3. Topological indices

2.3.1. Xu and atom type indices

Xu index, novel atom type index (*AI*) defined and described elsewhere [37–43], encode the molecular connectivity, charge information and individual contributions from atoms or groups in the molecules to the physicochemical properties were derived using the vertex-adjacency matrix, $A = [a_{ij}]_{\text{nxn}}$ and distance matrix, $D = [d_{ij}]_{\text{nxn}}$. For example, a_{ij} is 1, if vertices "*i*" and "*j*" are adjacent and if they are separated by more than one carbon in between a_{ij} will be zero. Similarly d_{ij} is the length of shortest path between vertex "*i*" and vertex "*j*" in molecular graph G, $G = [V, E]$, Where "*V*" represents the atoms of the molecule and "*E*" symbolizes bonds between pairs of atoms.

Fig. 1 depicts the molecular graph of a typical trialkyl phosphate, T2MBP, where each vertex is represented by a number as per the

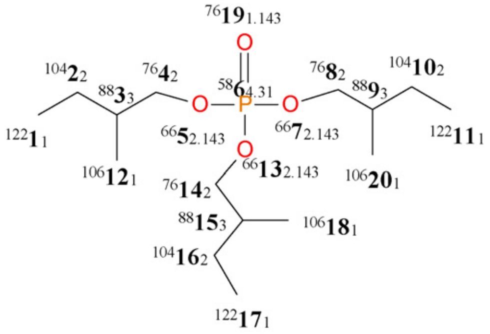

Fig. 1. Labeled molecular graph of T2MBP.

Table 2
Retention indices of trialkyl phosphates on different polar stationary phases.

Compound	Acronym	Apiezon L	SE-30	XE-60
Trimethyl phosphate	TMP	754.92	804.43	1392.25
Triethyl phosphate	TEP	939.34	952.26	1529.16
Tri-sec-butyl phosphate	TsBP	1339.44	1434.49	1857.40
Triisobutyl phosphate	TiBP	1371.44	1459.20	1877.10
Tri-sec-amyl phosphate	TsAP	1525.12	1629.63	1973.68
Tri n-butyl phosphate	TBP	1579.71	1665.94	2142.73
Tri-2-methyl butyl phosphate	T2MBP	1681.25	1762.85	2223.61
Triisoamyl phosphate	TiAP	1704.60	1770.08	2256.34
Tri n-amyl phosphate	TAP	1889.93	1892.61	2458.00
Tri n-hexyl phosphate	THP	2270.65	2278.27	2600.84

nomenclature rule of organic compounds, with a superscript and subscript representing the distance sum vector and vertex-degree, V^m, respectively. The modified *Xu* index, [40] where V^m is used in the calculation instead of V_i of *Xu* index, for T2MBP is calculated as:

$$Xu = 20^{1/2}\log\left[\frac{296713.532}{3317.162}\right] = 8.7276$$

The various atom indices of T2MBP are calculated as:

$$AI(-CH_3-) = AI(1)+AI(11)+AI(17)+AI(12)+AI(18)+AI(20) = 29.6225$$

$$AI(-CH_2-) = AI(2)+AI(4)+AI(8)+AI(10)+AI(14)+AI(16) = 36.0111$$

$$AI(\rangle CH-) = AI(3)+AI(9)+AI(15) = 24.0107$$

$$AI(-O-) = AI(5)+AI(7)+AI(13) = 11.4423$$

$$AI\left(\overset{\|}{\underset{|}{-P-}}\right) = AI(6) = 5.3708$$

$$AI\left(\overset{\|}{O}\right) = AI(19) = 2.9902$$

2.3.2. Steric effect index

Steric effect index [44,45] describes the bulkiness of the molecule and each of sub-sets encodes of weighted count which are incorporated into numerical indices and is expressed as: $SV_{ij} = \Sigma V_{ij}$ and $V_{ij} = (V_i \times V_j)^2$, where V_i and V_j are degree of vertex *i* and vertex *j* in C_i–C_j bond. For T2MBP, excluding the phosphate bonds, the SV_{ij} can be calculated as per the definition [45], as follows:

$$\begin{aligned}SV_{ij} = {} & (C_1\times C_2)^2+(C_2\times C_3)^2+(C_3\times C_4)^2+(C_4\times C_5)^2+(C_5\times C_6)^2\\ & +(C_6\times C_7)^2+(C_7\times C_8)^2+(C_3\times C_9)^2+(C_3\times C_{10})^2\\ & +(C_{10}\times C_{11})^2+(C_{11}\times C_{12})^2+(C_{12}\times C_{13})^2+(C_{11}\times C_{14})^2\\ & +(C_6\times C_{15})^2+(C_6\times C_{10})^2 = 343\end{aligned}$$

3. Results and discussion

3.1. Variation in retention indices on different polar stationary phase

Retention indices of the compounds under this study are found to increase with increasing polarity of the stationary phase whose structure is important for the retention behaviour exhibited by the solute. Apiezon L coated stationary phase possesses high molecular weight alkanes and its dominant interaction with trialkyl phosphates are non-specific hence resulting in low retention index values. SE-30 stationary phase is a polysiloxane polymer containing Si–O- and Si–C- linkages with methyl groups attached to silicon atoms, while XE-60 stationary phase has cyanoethyl methyl substituent attached to silicon atoms. The SE-30 stationary phase is non-polar with no polarizable and polar side chains and its interactions with solute molecules are non-specific that sequel the lower retention indices than XE-60 column. The specific interaction of XE-60 column with trialkyl phosphates is contributed by –CN groups. Therefore retention index on XE-60 column can be expected to be higher than those in SE-30 column. A noticeable change is observed in the retention index for a particular phosphate with varying polarity and most pronounced for XE-60 stationary phase and is listed in Table 2.

Table 3
Normal boiling points of trialkyl phosphates.

Compound	Normal boiling point (°C)		
	Literature [46]	From simple regression analysis	From multiple regression analysis
TMP	196	195.06	194.97
TEP	215	215.89	216.34
TsBP	–	261.06	260.75
TiBP	264	264.67	265.65
TsAP	–	282.02	282.74
TBP	289	288.19	285.45
T2MBP	–	299.65	298.20
TiAP	–	302.29	302.37
TAP	–	323.21	326.62
THP	–	366.12	365.02

Column: 4 m × 3.2 mm, Apiezon L, column oven: 100 °C for 2 min as initial and 225 °C for 25 min as final temperature, ramp: 1.5 °C/min.

Table 4
Topological indices of trialkyl phosphates.

Compound	Xu	$AI(\mathrm{CH_3}-)$	$AI(-\mathrm{CH_2}-)$	$AI(>\mathrm{CH}-)$	$AI(-\mathrm{O}-)$	$AI\left(\overset{ll}{\underset{l}{-\mathrm{P}-}}\right)$	$AI\left(\overset{ll}{\mathrm{O}}\right)$	SV_{ij}
TMP	3.3313	8.6766	0	0	8.9608	3.0388	2.3841	3
TEP	4.8562	11.3596	13.0419	0	9.4492	3.7097	2.5671	60
TsBP	7.3698	24.8875	17.867	17.689	10.3912	4.5889	2.7994	390
TiBP	7.4994	26.9716	13.1041	24.3345	10.7754	4.8552	2.8601	250
TsAP	8.6441	27.742	40.4848	18.164	11.0677	5.1222	2.9258	438
TBP	7.6644	16.6759	53.4258	0	11.0702	5.0755	2.9006	156
T2MBP	8.7276	29.6225	36.0111	24.0107	11.4423	5.3708	2.9902	343
TiAP	8.8354	31.9368	30.8961	31.3515	11.7457	5.5823	3.0382	298
TAP	8.9657	19.3207	80.9605	0	11.9918	5.7629	3.0735	204
THP	10.2172	21.9606	113.426	0	12.9454	6.4517	3.2484	252

3.2. Retention indices of trialkyl phosphates

In tri n-alkyl phosphates, the retention indices increase in a linear fashion with successive inclusion of carbon atoms which results in change in the structural parameters and electronic environment. It is obvious that retention of this system is facilitated by a linear conformation of phosphates. Steric hindrance and the presence of branching can affect the coplanarity of the molecule and make the approach the stationary phase difficult, thereby diminishing interactions resulting in lower value of retention index. Lower value of retention index of TsBP and TsAP is attributed to the prevention of phosphates getting a close contact with stationary phase thus reducing their interaction. Obviously, the contribution of the bulkiness of the molecule to the retention index is less and thus TBP is found to have a larger retention index than TsAP with a higher molecular weight due to strong interactions.

3.3. Evaluation of normal boiling point

The boiling points derived from the retention indices obtained in this study and literature values [46] are summarized in Table 3. While normal boiling point (T_{bp}) values for TsBP, TsAP, T2MBP TiAP, TAP and THP were determined from their respective retention index value from the linear regression line obtained by plotting the *RI* versus the literature values of TMP, TEP, TiBP and TBP. It can be observed that normal boiling point of homologous trialkyl phosphates increase monotonically with increasing carbon atoms in the alkyl chain. Obviously, number of carbon atoms overwhelmingly influences the normal boiling point in homologues. It can also be seen that the boiling point is less for branched phosphates and among the branched ones the phosphates which are branched near the alkoxy carbon have still lower boiling point. This feature can be explained by the intermolecular distance and the packing density in the liquids, which varies in the order TBP < TiBP < TsBP and thus the boiling points vary in the reverse order.

3.4. Simple linear regression

A plot of available normal boiling point of trialkyl phosphates as a function of retention index is illustrated in Fig. 2 typically for injections in Apiezon L stationary phase. The line drawn in the figure was computed by simple linear regression analysis using the value of normal boiling points of TMP, TEP, TiBP and TBP as reference standards and is represented by the following equation:

$$T_{\mathrm{bp}}(\text{Apiezon L}) = (RI \times 0.1129) + 109.8368 \qquad R = 0.9998, \quad \mathrm{SD} = 1.1756 \tag{2}$$

Using the above equation and the retention indices, the normal boiling points of the phosphates, TsBP, TAP, TiAP, TsAP, T2MBP and THP have been derived and are listed in Table 3. Similar equations for the other stationary phases are given below,

$$T_{\mathrm{bp}}(\text{SE-30}) = (RI \times 0.1050) + 112.8028 \qquad R = 0.9989, \quad \mathrm{SD} = 2.4676 \tag{3}$$

$$T_{\mathrm{bp}}(\text{XE-60}) = (RI \times 0.1260) + 22.4350 \qquad R = 0.9963, \quad \mathrm{SD} = 4.5073 \tag{4}$$

3.5. Multiple linear regression and structural interpretation on normal boiling point

Topological indices such as *Xu* index, atom type indices and steric effect index were computed for trialkyl phosphates and are listed in Table 4. Multiple linear regressions (MLR) analysis based on a combination of the *Xu* index, atom type indices and steric effect index was performed to correlate normal boiling point of trialkyl phosphates and the following regression equation was obtained,

$$\begin{aligned} T_{\mathrm{bp}} = {} & -2407.1929 + [Xu(40.5981)] - [AI(-\mathrm{CH_3}-)(7.5112)] \\ & - [AI(-\mathrm{CH_2}-)(1.44)] + [AI(\rangle \mathrm{CH}-)(0.0466)] \\ & + [AI(-\mathrm{O}-)(152.6782)] - \left[AI\left(\overset{ll}{\underset{l}{-\mathrm{P}-}}\right)(385.11)\right] \\ & + \left[AI\left(\overset{ll}{\mathrm{O}}\right)(979.03)\right] + [SV_{ij}(0.0528)] \end{aligned}$$

The positive values in the regression coefficient indicate that the indicated descriptor contributes positively to the value of normal boiling point, whereas negative values indicate negative contribution. Thus, higher $AI\left(\overset{ll}{\underset{l}{-\mathrm{P}-}}\right)$, $AI(-\mathrm{CH_3}-)$, and $AI(-\mathrm{CH_2}-)$ will decrease while higher (Xu), $AI(>\mathrm{CH}-)$, $AI(-\mathrm{O}-)$, $AI\left(\overset{ll}{\mathrm{O}}\right)$ and SV_{ij} tend to increase the extent of normal boiling point of

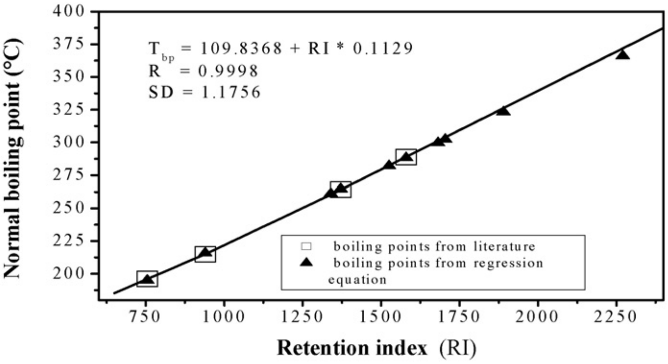

Fig. 2. Variation of the normal boiling point with retention index.

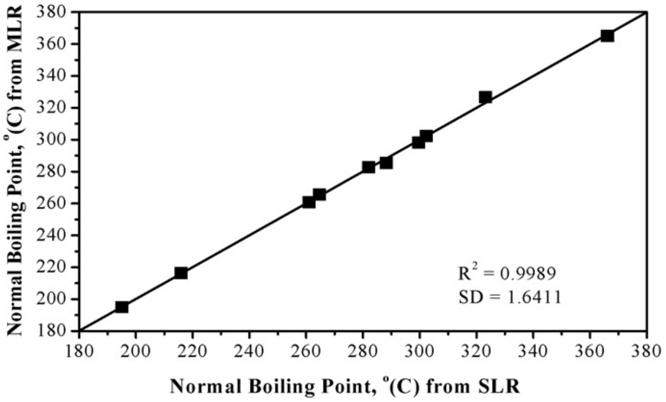

Fig. 3. Correlation between normal boiling points determined through simple linear regression and multiple linear regression.

trialkyl phosphates. The order of significance of the descriptors is: $AI\left(\overset{ll}{\mathrm{O}}\right) > AI(–\mathrm{O}–) > Xu > SV_{ij} > AI(\rangle CH-) > AI(–\mathrm{CH_2}–) > AI(–\mathrm{CH_3}) > AI\left(\overset{ll}{\underset{l}{–\mathrm{P}–}}\right)$. The results also reveal that the normal boiling points of trialkyl phosphates are predominantly decided by number of oxygen atoms, molecular size and degree of branching. It is found that *Xu* index also is a major contributor to normal boiling point, since it contains information on molecular connectivity and charge. Steric effect index characterizing bulkiness of the molecule has minor contribution to normal boiling point for linear alkyl chain phosphates. It is apparent that branching prevents close contact with neighboring molecules in space and varied with degree of branching for molecules with same number of non-hydrogen atoms. It can be observed that the value of $AI(–\mathrm{CH_3}–)$ reveals that the relative contribution from peripheral methyl group keeps much steady for isoalkyl phosphates than others. The atom type index, $AI(>\mathrm{CH}–)$, are obviously related to the counts of $>\mathrm{CH}–$ group in a molecule, which is a crude measure of branching and decrease in the order: iso > inside > secondary > linear alkyl phosphates and zero contribution of $AI(>\mathrm{CH}–)$ index in linear alkyl chain phosphates reflects its unbranching carbon backbone.

The magnitude of the correlation coefficient of the multiple linear regressions reiterates that the topological indices can be effectively used to predict the normal boiling point and Fig. 3 depicts a linear relationship exists between estimated and predicted normal boiling points.

4. Conclusions

Measurement of retention index is reliable, simple and fast method for estimating normal boiling points of trialkyl phosphates. Highly non-polar stationary phases, i.e., Apiezon L yield a better correlation between retention indices and normal boiling point than those which exhibit slightly polar nature. The topological indices help to predict normal boiling points of trialkyl phosphates through multiple linear regressions.

Acknowledgement

The authors gratefully acknowledge Dr. A. Suresh for providing synthesized trialkyl phosphates.

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