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Solid vapor pressure for five heavy PAHs via the Knudsen effusion method

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Abstract

Polycyclic aromatic hydrocarbons (PAHs) are compounds resulting from incomplete combustion and many fuel processing operations, and they are commonly found as subsurface environmental contaminants at sites of former manufactured gas plants. Knowledge of their vapor pressures is the key to predict their fate and transport in the environment. The present study involves five heavy PAHs, *i.e.* benzo[*b*]fluoranthene, benzo[*k*]fluoranthene, benzo[*ghi*]perylene, indeno[1,2,3-*cd*]pyrene, and dibenz[*a,h*]anthracene, which are all as priority pollutants classified by the US EPA. The vapor pressures of these heavy PAHs were measured by using Knudsen effusion method over the temperature range of 364 K to 454 K. The corresponding values of the enthalpy of sublimation were calculated from the Clausius-Clapeyron equation. The enthalpy of fusion for the 5 PAHs was also measured by using differential scanning calorimetry and used to convert earlier published sub-cooled liquid vapor pressure data to solid vapor pressure in order to compare with the present results. These adjusted values do not agree with the present measured actual solid vapor pressure values for these PAHs, but there is good agreement between present results and other earlier published sublimation data.

Keywords

polycyclic aromatic hydrocarbon; vapor pressure; enthalpy of sublimation; enthalpy of fusion; Knudsen effusion method

1 Introduction

Polycyclic aromatic hydrocarbons (PAHs) are one of the main classes of persistent organic pollutants which occur naturally in petroleum and result from incomplete combustion and many fuel processing operations. Sixteen PAHs are listed as priority pollutants by the US Environmental Protection Agency (US EPA). Health effects are of concern due to their persistence, toxic and carcinogenic properties. The thermodynamic properties of PAHs have been widely studied for more than 50 years [1–22].

Vapor pressure is a fundamental property which is the key to predict the fate and transport of a substance in the environment. Many experimental techniques have been developed to measure the vapor pressure of PAHs, such as the Knudsen effusion method [9–11, 17, 21], the generator column–HPLC method [5], the gas saturation method [19], the electronic

manometry method [23], and the GC-retention time method [14, 20]. Several compendia of vapor pressures for PAHs have also been published, which detail many correlations and also uncertainties in current experimental data [1–4]. However, many of the previous studies have focused on light PAHs, and only limited vapor pressure data exist for heavy PAHs. This is especially true for benzo[*b*]fluoranthene, benzo[*k*]fluoranthene, benzo[*ghi*]perylene, indeno[1,2,3-*cd*]pyrene, and dibenz[*a,h*]anthracene, of which all are US EPA priority pollutants. The heavier PAHs are more persistent than the lighter PAHs and tend to have greater carcinogenic and other chronic impact potential.

In this study, the Knudsen effusion technique was used to measure the solid vapor pressures, their temperature dependence, and enthalpies of sublimation for five heavy PAHs, *i.e.* benzo[*b*]fluoranthene, benzo[*k*]fluoranthene, benzo[*ghi*]perylene, indeno[1,2,3-*cd*]pyrene and dibenz[*a,h*]anthracene. Additionally, the enthalpies of fusion, phase change of these PAHs, have also been studied by using differential scanning calorimetry.

2 Materials and methods

2.1 Materials

The five heavy polycyclic aromatic hydrocarbons that were examined fall in the molar mass (*M*) range from 252 g·mol⁻¹ to 278 g·mol⁻¹. They were purchased from TCI and Aldrich with minimum mass fraction purity 0.95, as detailed in table 1. They were used in the measurements without further purification.

2.2 Enthalpies of fusion

The enthalpies of fusion were measured using a TA instruments 2910 differential scanning calorimeter (DSC). A 1 mg to 3 mg sample was placed into a hermetically sealed DSC pan and this was scanned in heating mode at a heating rate of 10 K·min⁻¹. The uncertainty in the DSC measurement is about ± 5 J·g⁻¹. The calibration of DSC consists of two procedures, baseline calibration and temperature calibration. The baseline calibration minimizes the temperature fluctuation in the heating process to permit the correct conversion of temperature difference to heat flow. This procedure is done by removing the pans from the DSC cell with the purge gas flow set at desired flow rate, 50 cm³·min⁻¹. The baseline obtained is used to calculate the slope and offset values. The temperature calibration uses standard indium which allows establishing both an accurate melting temperature and enthalpy. More details of this technique can be found in a previous publication [24].

2.3 Vapor pressure

The Knudsen effusion technique derives from Knudsen's 1909 Kinetic Theory of Gases. The Knudsen effusion method is an indirect measurement technique based on the molecular effusion of a vapor through an orifice into a high vacuum chamber and is generally used to measure the vapor pressure of low volatility substances. The present implementation of the Knudsen effusion method is described in a previous publication [24]. Samples were placed inside effusion cells prepared from steel shim stock. The cells were sealed except for a single, circular orifice (0.61 ± 0.02) mm in diameter, and then placed on one arm of a continuously recording microbalance in a high vacuum chamber. The pressure inside of the chamber was reduced to 10⁻⁴ Pa in the experiments. The measurements were made under isothermal conditions by using a type K thermocouple located above the effusion cell. More details of this technique may be found in Goldfarb *et al.* [9] and Oja *et al.* [17].

3 Results and discussion

DSC was used to study the enthalpies of fusion of these five PAHs and the data are compared with literature values in table 2. The value for benzo[*b*]fluoranthene is within the literature range, while the values for benzo[*k*]fluoranthene, benzo[*ghi*]perylene and dibenz[*a,h*]anthracene are about 0.2 kJ·mol⁻¹ to 2.3 kJ·mol⁻¹ lower than the published range of literature values. The enthalpy of fusion for indeno[1,2,3-*cd*]pyrene in this study is about 1.4 kJ·mol⁻¹ higher than literature values. Bearing in mind the measurement uncertainty of $\pm 5 \text{ J}\cdot\text{g}^{-1}$, the present measured values would have an inherent uncertainty of 1.3 kJ·mol⁻¹ to 1.4 kJ·mol⁻¹.

The enthalpies of fusion data were used to correct the sub-cooled state vapor pressures to real solid vapor pressures (see below).

Table 3 presents the raw data obtained in the present experiment using the Knudsen effusion method. The reference compound anthracene was employed to test periodically the performance of the Knudsen effusion apparatus and the results are in good agreement with literature values [5, 7, 9, 12] (see Figure 1(a)). These data were used to calculate the enthalpy ($\Delta_{\text{sub}}H$) and entropy ($\Delta_{\text{sub}}S$) of sublimation, and vapor pressure at $T = 298.15 \text{ K}$ using the Clausius-Clapeyron equation, integrated assuming a constant enthalpy of sublimation,

$$\ln \frac{P}{P_0} = - \frac{\Delta_{\text{sub}}H}{R} \left(\frac{1}{T} - \frac{1}{T_0} \right)$$

where R is the universal gas constant, T is the absolute temperature of the sample ($T < T_{\text{fus}}$), and P_0 and T_0 are values at a related reference condition.

Table 4 presents the results of fitting the data with the Clausius-Clapeyron equation (Eq. (1)) along with the statistical significance of these results. The enthalpy of sublimation value presented here is calculated from the slope of the Clausius-Clapeyron equation for the temperature range indicated in table 3. The vapor pressure at $T = 298.15 \text{ K}$ was also calculated by using Eq. (1) and the entropy of sublimation from $\Delta_{\text{sub}}H = T \Delta_{\text{sub}}S$. The enthalpies of sublimation of four of these compounds have been summarized in a review [25]. The enthalpy of sublimation values were compared with these earlier published values and the data are generally in good agreement.

As noted, few thermodynamic data are available in the literature for these heavy PAHs, especially solid vapor pressures. The solid phase sublimation data can be supplemented by published sub-cooled liquid vapor pressures (P_L). These can be converted to solid vapor pressure (P_S) at a given temperature by

$$\ln P_L / P_S = \Delta_{\text{fus}}S (T_{\text{fus}} - T) / RT$$

where T_{fus} is the melting temperature, $\Delta_{\text{fus}}S$ is the entropy of fusion, and $\Delta_{\text{fus}}S = \Delta_{\text{fus}}H / T_{\text{fus}}$. The reliability of this conversion methods for PAH vapor pressures was established by comparing the converted vapor pressures of anthracene and phenanthrene [14, 20] to available actual vapor pressure values [9, 17], as displayed in Figure 1(b). The converted data are in good agreement with actual values. Additionally, the sub-cooled vapor pressures for these two light PAHs measured by Lei *et al.* [14] and Odabasi *et al.* [20] agree fairly

well with each other. Hence these data confirm the general validity of an approach based on Eq. (2).

Figure 2 shows the results for benzo[*b*]fluoranthene compared to available sub-cooled vapor pressure data [14; 20]. While an enthalpy of sublimation has been published for this compound [22], the underlying sublimation vapor pressure data have not been published in the open literature. The present measurements provide an enthalpy of sublimation for benzo[*b*]fluoranthene of $(118.8 \pm 0.8) \text{ kJ}\cdot\text{mol}^{-1}$, which may be compared with the literature value $119.2 \text{ kJ}\cdot\text{mol}^{-1}$ [22]. The enthalpies of vaporization for sub-cooled benzo[*b*]fluoranthene liquid estimated by Lei *et al.* [14] and Odabasi *et al.* [20] were $89.6 \text{ kJ}\cdot\text{mol}^{-1}$ and $98.6 \text{ kJ}\cdot\text{mol}^{-1}$, respectively. After the adjustment by Eq. (2), the enthalpies of sublimation estimated by Eq. (2) are $107.9 \text{ kJ}\cdot\text{mol}^{-1}$ and $116.9 \text{ kJ}\cdot\text{mol}^{-1}$, respectively. The value from Odabasi *et al.* is close to the value presently obtained. Additionally, the vapor pressure data obtained in the present measurements appear to fall between the two adjusted vapor pressure data sets. Data converted from Lei *et al.* are about 70 % lower than the actual measured solid vapor pressure, whereas the data converted from Odabasi *et al.* are about 45 % higher than the values obtained in the present study.

Figure 3 provides data on benzo[*k*]fluoranthene, which has the same molar mass as benzo[*b*]fluoranthene. Diogo and Minas also used the Knudsen effusion method to measure the vapor pressure of benzo[*k*]fluoranthene [26] and Stephenson and Malanowski [27] reported values, the source of which was not given. The enthalpy of sublimation derived from the data of Diogo and Minas, $119.9 \text{ kJ}\cdot\text{mol}^{-1}$, is within the range of this study, $(121.5 \pm 3.3) \text{ kJ}\cdot\text{mol}^{-1}$, while their vapor pressure data are about 8 % to 30 % higher than the values obtained in this study (see Figure 3(b)). The vapor pressures and enthalpy of sublimation estimated from Lei *et al.* [14] are again lower than the vapor pressure and enthalpy of sublimation obtained in this study, whereas those obtained from the measurements of Odabasi *et al.* are higher than the present values. The solid vapor pressure data from Stephenson and Malanowski's handbook [27] and estimated from Odabasi *et al.* [20] differ from our study by about 15 % to 50 % within the temperature range of 384 K to 424 K, whereas the enthalpies of sublimation value estimated are about $10 \text{ kJ}\cdot\text{mol}^{-1}$ and $4 \text{ kJ}\cdot\text{mol}^{-1}$ respectively higher than the value obtained in this study.

The vapor pressure for benzo[*ghi*]perylene is shown in figure 4. The solid state vapor pressures of this compound were also measured by Murray and Pottiel [16], and Wakayama and Inokuchi [21] using the Knudsen effusion method. The values reported by Murray and Pottiel are about 35 % to 55 % higher than those of this study in the temperature range of 399 K to 454 K, while the data obtained in the measurements of Wakayama and Inokuchi are about 30 % to 50 % lower than the present values (Figure 4(b)). However, both of them reported enthalpies of sublimation, $127.8 \text{ kJ}\cdot\text{mol}^{-1}$ and $126.0 \text{ kJ}\cdot\text{mol}^{-1}$, respectively, are close to the value obtained in this study, $(128.0 \pm 2.0) \text{ kJ}\cdot\text{mol}^{-1}$. Just as in the case of benzo[*b*]fluoranthene and benzo[*k*]fluoranthene, the results estimated from Lei *et al.* fall below those from the present study, whereas those of Odabasi *et al.* fall above. The enthalpy of sublimation estimated from the data set of Odabasi *et al.*, $126.1 \text{ kJ}\cdot\text{mol}^{-1}$, is within experimental error of that from the present measurement, $(128.0 \pm 2.0) \text{ kJ}\cdot\text{mol}^{-1}$, and agrees reasonably well with the other earlier reported values.

Just as in the case for benzo[*b*]fluoranthene, only sub-cooled vapor pressure data have been published for indeno[1,2,3-*cd*]pyrene (Figure 5). The estimated enthalpy of sublimation calculated from the GC-retention time method [20] and our enthalpy of fusion, $131.8 \text{ kJ}\cdot\text{mol}^{-1}$, is in this case about $7 \text{ kJ}\cdot\text{mol}^{-1}$ higher than the value from present actual sublimation experiments, whereas the vapor pressures converted from the data of Odabasi *et al.* are about two times higher than the presently measured solid vapor pressures.

Dibenz[*a,h*]anthracene with the molar mass $278.35 \text{ g}\cdot\text{mol}^{-1}$ is the largest PAH on the list of 16 priority pollutants. Figure 6 presents the data for dibenz[*a,h*]anthracene. The vapor pressure and enthalpy of sublimation data obtained here within the temperature range of 399 K to 449 K agree well with data published by de Kruif [6], who also employed an effusion technique. However, the values from Wakayama and Inokuchi are 3 to 5 times lower than the present values, even though their reported enthalpy of sublimation, $142.0 \text{ kJ}\cdot\text{mol}^{-1}$ is within the range of this study, $(138.1 \pm 5.6) \text{ kJ}\cdot\text{mol}^{-1}$. Once again, the GC-retention time method led to lower or higher estimates of the solid phase vapor pressures than those directly measured in this work.

It is interesting to note that the enthalpies of sublimation and vapor pressures for these five PAHs are very different, even though molar mass for these PAHs are either the same or very close. The thermochemical properties of PAHs depend on the details of their molecular structure and interaction.

The widely used GC-retention time method can be used to estimate the vapor pressure and enthalpy of sublimation for light PAHs such as anthracene, but its application to heavy PAHs seems to lead to somewhat variable results. The different vapor pressures estimated from the studies of Lei *et al.* and Odabasi *et al.* may be due to the use of different GC columns with different non-polar stationary phases [20]. In fact, the results here suggest that values reported as “sub-cooled liquid state” vapor pressures might sometimes actually be closer to actual solid state sublimation vapor pressures. The reasons for this are not clear at this time.

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FIGURE 1.

Plot of vapor pressure against reciprocal temperature as a measure of system performance by using anthracene and solid vapor pressures of anthracene and phenanthrene compared to available literature values [14, 20] obtained by using GC-retention time method: (a) ●, anthracene P_S this study; — — —, anthracene P_S from Bender *et al.* [7]; — — —, anthracene P_S from Sonnefeld *et al.* [5]; — - — —, anthracene P_S from Hansen and Eckert [12]; — — —, anthracene P_S from Goldfarb and Suuberg [9]. (b) Δ, phenanthrene P_S ; ●, anthracene P_S [9]; — — —, phenanthrene or anthracene P_L from Lei *et al.* [14] and Odabasi *et al.* [20]; — — —, phenanthrene P_S estimated from P_L [14, 20]; — - — —, anthracene P_S estimated from P_L [14, 20].

FIGURE 2.

Plot of vapor pressure against reciprocal temperature for benzo[*b*]fluoranthene obtained by using the Knudsen effusion method compared to available literature values [14; 20]: ●, P_S this study; thin solid line, P_L from Lei *et al.* [14]; heavy solid line, P_S estimated from P_L [14]; thin dashed line, P_L from Odabasi *et al.* [20]; heavy dashed line, P_S estimated from P_L [20].

FIGURE 3.

Plot of vapor pressure against reciprocal temperature for benzo[*k*]fluoranthene obtained by using the Knudsen effusion method compared to available literature values: (a) ●, P_S this study; ×, P_S from the handbook of Stephenson and Malanowski [27]; Δ, P_S from Diogo and Minas [26]; thin solid line, P_L from Lei *et al.* [14]; heavy solid line, P_S estimated from P_L [14]; thin dashed line, P_L from Odabasi *et al.* [20]; heavy dashed line, P_S estimated from P_L [20]. (b) —●—, P_S this study; —×—, P_S from Stephenson and Malanowski's handbook [27]; —Δ—, P_S from Diogo and Minas [26].

FIGURE 4.

Plot of vapor pressure against reciprocal temperature for benzo[ghi]perylene obtained by using the Knudsen effusion method compared to available literature values: (a) $\bullet$, P_S this study; $\times$, P_S from Murray and Pottiel [16]; Δ , P_S from Wakayama and Inokuchi [21]; thin solid line, P_L from Lei *et al.* [14]; heavy solid line, P_S estimated from P_L [14]; thin dashed line, P_L from Odabasi *et al.* [20]; heavy dashed line, P_S estimated from P_L [20]. (b) $-\bullet-$, P_S this study; $-\times-$, P_S from Murray and Pottiel [16]; $-\Delta-$, P_S from Wakayama and Inokuchi [21].

FIGURE 5.

Plot of vapor pressure against reciprocal temperature for indeno[1,2,3-*cd*]pyrene obtained by using the Knudsen effusion method compared to available literature values: ●, P_S this study; thin dashed line, P_L from Odabasi *et al.* [20]; heavy dashed line, P_S estimated from P_L [20].

FIGURE 6.

Plot of vapor pressure against reciprocal temperature for dibenz[*a,h*]anthracene obtained by using the Knudsen effusion method compared to available literature values: $\bullet$, P_S this study; $\times$, P_S from de Kruif [6]; Δ , P_S from Wakayama and Inokuchi [21]; thin solid line, P_L from Lei *et al.* [14]; heavy solid line, P_S estimated from P_L [14]; thin dashed line, P_L from Odabasi *et al.* [20]; heavy dashed line, P_S estimated from P_L [20].

Table 1

Polycyclic aromatic hydrocarbons examined.

CAS Reg. No.	Compound	Min. Purity	M/ g·mol ⁻¹	T _{fus} /K [3]	Molecular structure
205-99-2	benzo[<i>b</i>]fluoranthene	0.95	252.31	441.15
207-08-9	benzo[<i>k</i>]fluoranthene	0.98	252.31	490.15
191-24-2	benzo[<i>ghi</i>]perylene	0.97	276.33	545.65
193-39-5	indeno[1,2,3- <i>cd</i>]pyrene	0.99+	276.33	435.15
53-70-3	dibenz[<i>a,h</i>]anthracene	0.95	278.35	542.65

Table 2

Enthalpy of fusion. Overview of the experimental data range ($\Delta_{\text{fus}}H(\text{lit.})$) [1; 25] and the DSC study here ($\Delta_{\text{fus}}H(\text{DSC})$) for the 5 PAHs.

Compound	$\Delta_{\text{fus}}H(\text{lit.})/\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_{\text{fus}}H(\text{DSC})/\text{kJ}\cdot\text{mol}^{-1}$
benzo[<i>b</i>]fluoranthene	18.3 – 20.9	18.3
benzo[<i>k</i>]fluoranthene	27.4 – 34.2	26.5
benzo[<i>ghi</i>]perylene	16.5 – 18.3	16.3
indeno[1,2,3- <i>cd</i>]pyrene	17.8 – 21.5	22.9
dibenz[<i>a,h</i>]anthracene	26.8 – 31.2	24.5

Table 3

Summary of vapor pressure obtained via Knudsen effusion method.

<i>T/K</i>	<i>P/Pa</i>	<i>T/K</i>	<i>P/Pa</i>	<i>T/K</i>	<i>P/Pa</i>
benzo[<i>b</i>]fluoranthene					
364.1	4.70E-03	384.2	3.95E-02	397.1	1.31E-01
369.3	8.12E-03	387.2	5.40E-02	399.1	1.59E-01
374.2	1.46E-02	389.1	6.22E-02	404.1	2.30E-01
377.2	1.90E-02	392.1	8.51E-02	409.0	3.56E-01
379.2	2.41E-02	394.2	1.01E-01	414.1	5.33E-01
382.2	3.21E-02				
benzo[<i>k</i>]fluoranthene					
384.2	1.63E-02	399.1	5.62E-02	411.0	1.57E-01
389.2	2.42E-02	404.0	8.86E-02	419.0	3.83E-01
394.1	3.62E-02	409.0	1.36E-01	424.0	5.57E-01
benzo[<i>ghi</i>]perylene					
399.1	4.16E-03	419.0	2.83E-02	439.0	1.38E-01
404.0	7.00E-03	424.0	4.36E-02	441.0	2.07E-01
409.0	1.15E-02	429.0	6.54E-02	449.1	3.03E-01
414.4	1.79E-02	434.1	1.04E-01	454.1	4.32E-01
indeno[1,2,3- <i>cd</i>]pyrene					
384.1	5.38E-03	399.2	2.19E-02	414.1	8.53E-02
389.1	7.96E-03	404.1	3.28E-02	419.1	1.33E-01
394.2	1.30E-02	409.1	5.33E-02	424.1	2.01E-01
dibenz[<i>a,h</i>]anthracene					
399.2	5.11E-03	419.1	3.95E-02	439.1	1.74E-01
404.0	5.53E-03	424.2	5.45E-02	444.1	2.80E-01
409.1	9.22E-03	429.2	8.89E-02	449.1	3.69E-01
414.0	1.39E-02	434.2	1.12E-01		

Table 4

Application of Clausius-Clapeyron equation to present vapor pressure data.

Compound	Temp range/K	$\Delta_{\text{sub}}H/\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_{\text{sub}}S/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$ (298.15K)	P/Pa (298.15K)
benzo[<i>b</i>]fluoranthene	364 – 414	118.8 ± 0.8	398.5 ± 2.7	8.40E-07
benzo[<i>k</i>]fluoranthene	384 – 424	121.5 ± 3.3	407.5 ± 11.1	2.47E-07
benzo[<i>ghi</i>]perylene	399 – 454	128.0 ± 2.0	429.3 ± 6.7	9.37E-09
indeno[<i>1,2,3-cd</i>]pyrene	384 – 424	124.7 ± 1.5	418.2 ± 5.0	6.44E-08
dibenz[<i>a,h</i>]anthracene	399 – 449	138.1 ± 5.6	463.2 ± 18.8	3.07E-09