



Estimating subcooled liquid vapor pressures and octanol-air partition coefficients of polybrominated diphenyl ethers and their temperature dependence

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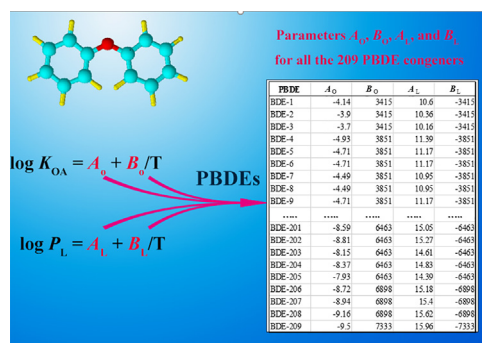
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HIGHLIGHTS

- A simple equation to relate $\log K_{OA}$ and $\log P_L$ ($\log K_{OA} = -\log P_L + 6.46$)
- Internal energy of phase transfer between octanol and air for all 209 PBDE congeners
- Clausius-Clapeyron coefficients of A_L & B_L ($\log P_L = A_L + B_L/T$) and A_O & B_O ($\log K_{OA} = A_O + B_O/T$) for all 209 PBDE congeners

GRAPHICAL ABSTRACT



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ABSTRACT

Both subcooled liquid vapor pressure (P_L) and octanol-air partition coefficient (K_{OA}) are widely used as descriptors to predict gas-particle partitioning behavior of semi-volatile organic compounds (SVOCs), such as polybrominated diphenyl ethers (PBDEs). These two descriptors are functions of temperature, which are expressed as the Clausius-Clapeyron equations with the coefficients A_L and B_L for P_L ($\log P_L = A_L + B_L/T$) and A_O and B_O for K_{OA} ($\log K_{OA} = A_O + B_O/T$), where T is temperature in K. In this study, a simple equation to relate $\log K_{OA}$ and $\log P_L$ ($\log K_{OA} = -\log P_L + 6.46$) was derived, which also links the coefficients of A_L & B_L and A_O & B_O . Regression analysis of published data of internal energy ΔU_{OA} for 22 PBDE congeners with their mole mass was made, leading a regression equation to calculate the internal energy for all 209 PBDE congeners. Three datasets of $\log K_{OA}$ at 25 °C for all 209 PBDE congeners were evaluated; the one with the best match with experimentally measurements was selected. Using the datasets and equations described above, we calculated the values of Clausius-Clapeyron coefficients A_O & B_O and A_L & B_L for all 209 PBDE congeners at the following steps. First, B_O was computed using the values of ΔU_{OA} . Next, we calculated the values of A_O using the values of B_O and the values of $\log K_{OA}$ at 25 °C. Finally, the values of the parameter A_L and B_L were determined for all 209 PBDE congeners. Results are in consistent with data available in the literature and the accuracy of the data were also evaluated. With these Clausius-Clapeyron coefficients, the values of P_L and K_{OA} at any environmentally relevant temperature

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can be calculated for all 209 PBDE congeners, and thus provides a quick reference for environmental monitoring and modeling of PBDEs.

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1. Introduction

Polybrominated diphenyl ethers (PBDEs), as a group of important brominated flame retardants (BFRs), are a family of halogenated organic compounds with a common structure of two benzene rings. There are 209 congeners, distinguished by both the number of bromine atoms (1–10) and their placement (i.e., ortho-, meta-, and para-position). Widely used as flame-retardant additives in a wide variety of industries, PBDEs have three major commercial products: commercial pentabromodiphenyl ether (ComPentaBDE), commercial octabromodiphenyl ether (ComOctaBDE), and commercial decabromodiphenyl ether (ComDecaBDE) (Shaw and Kannan, 2009).

All the three commercial products are highly persistent in the environment, bioaccumulative, and have a potential for long-range environmental transport. There has been evidence of their toxic effects in wildlife, including mammals, and these chemicals have been detected in humans throughout the world (www.pops.int). As a result, ComPentaBDE and ComOctaBDE were added as new members of persistent organic pollutants (POPs) in the Stockholm Convention at the fourth Conference of the Parties (COP-4) held in May 2009 (www.pops.int). ComDecaBDE was proposed to be listed in Annexes A, B and C to the Stockholm Convention on POPs in 2013, and listed as a new member of POPs in 2016 (<http://chm.pops.int/>).

Atmospheric transport is a major mechanism of moving SVOCs, including PBDEs, from source regions to other remote places, including the Arctic and Antarctic, where these chemicals have never been produced and used (Barrie et al., 1992; Eckhardt et al., 2007; Li and Bidleman, 2003; Li et al., 1998; MacDonald et al., 2000). The gas/particle (G/P) partitioning of SVOCs is an important process that primarily governs their atmospheric fate, since wet and dry depositions and other processes act differently on gaseous and particulate SVOCs, thus affecting the efficiency and scope of their long-range atmospheric transport and fate (Bidleman, 1988). The G/P partition quotient of SVOCs, K_P , is commonly defined as (Yamasaki et al., 1982; Li et al., 2015)

$$K_P = (C_P/TSP)/C_G \quad (1)$$

where C_G and C_P ($\text{pg} \cdot \text{m}^{-3}$ in air) are concentrations of gaseous and particle-bound SVOCs, respectively, and TSP ($\mu\text{g} \cdot \text{m}^{-3}$) is the concentration of total suspended particle, thus K_P has a unit of $\text{m}^3 \mu\text{g}^{-1}$.

K_P of a SVOC in environment can be determined directly from their concentrations in air and on particles, but also estimated indirectly from other physicochemical properties of the substance. Both subcooled liquid vapor pressure (P_L) and octanol–air partition coefficient (K_{OA}) are widely used as descriptors to predict G/P partitioning behavior of SVOCs, such as PBDEs. Based on monitoring data, it is often found that K_P of an SVOC generally follows a log-linear relationship with P_L (Pankow, 1987; Pankow and Bidleman, 1991; Pankow and Bidleman, 1992) and K_{OA} (Finizio et al., 1997; Harner and Bidleman, 1998; Pankow, 1998) under ambient temperatures and prevailing particle characteristics and concentrations. Logarithm relationships between K_P and P_L & K_{OA} can be expressed as

$$\log K_P = m_L \log P_L + b_L \quad (2)$$

and

$$\log K_P = m_O \log K_{OA} + b_O \quad (3)$$

where m_L , m_O , b_O and b_L are empirical coefficients derived from

regressions, which vary with environmental conditions such as temperatures (Goss and Schwarzenbach, 1998).

Recently, Li and Jia (2014) found that m (m_L and m_O) and b (b_L and b_O) can be predicted with ambient air temperature ranged from -22 to 38 °C for 11 PBDE congeners, including BDE-17, -28, -47, -66, -85, -99, -100, -138, -153, -154, and -183:

$$m = m_O = -m_L = -2.74 + 0.011T \quad (4)$$

and

$$b_O = 41.88 - 0.135T \quad (5a)$$

$$b_L = 11.649 - 0.054T \quad (5b)$$

where T is ambient temperature with the unit of K.

Both P_L and K_{OA} are functions of temperature as expressed by the Clausius-Clapeyron equations. The equations for P_L (Tittlemier et al., 2002) and K_{OA} (Harner and Shoeib, 2002) are in the forms of

$$\log P_L = A_L + B_L/T \quad (6)$$

and

$$\log K_{OA} = A_O + B_O/T \quad (7)$$

Indicating by the above two equations and Eqs. (2) and (3), the Clausius-Clapeyron coefficients A_L and B_L for P_L and A_O and B_O for K_{OA} are important in studying G/P partitioning behavior of SVOCs. With these parameters, we are able to predict the variations of $\log P_L$ and $\log K_{OA}$ as functions of temperature. Unfortunately, these parameters are available for only a few PBDE congeners from some sources, which are listed in Table S1, Supplementary data; and available data are listed in Table S2 for A_L and B_L and Table S3, SI for A_O and B_O . Relationships between P_L of PBDEs and temperature (through the values of the parameter A_L and B_L) have been determined by Wong et al. (2001) with a gas chromatographic retention time technique for 23 PBDE congeners and by Tittlemier et al. (2002) using both the gas chromatography-retention time and generator column techniques for 14 PBDE congeners (Table S2). Relationship between K_{OA} and temperature (through the values of the parameter A_O and B_O) have been determined by Harner and Shoeib (2002) using the generator column technique for 13 PBDE congeners (Table S3) over the temperature range of 15 – 45 °C.

While both P_L and K_{OA} can be used to predict G/P partition of SVOCs, predictability based on the two parameters is about the same. Xiao and Wania (2003) compiled and evaluated a large dataset of P_L and K_{OA} for several sets of non-polar SVOCs, including PBDEs, and concluded that it is impossible to judge one parameter being better than the other. This is because P_L and K_{OA} obtained at the same temperature for any given compound are strongly correlated as given by (Xiao and Wania (2003)

$$\log K_{OA} = (-0.98784 \pm 0.00584) \log P_L + (6.6914 \pm 0.0171) \quad (8)$$

($R = 0.996$)

It was found that P_L and K_{OA} can be interconverted using the above equation with bias less than one order of magnitude (Xiao and Wania, 2003).

Harner and Bidleman (1996) studied the relationship between $\log P_L$ and $\log K_{OA}$ at $+20$ °C for polychlorinated biphenyls congeners containing two to seven Cl atoms. Different regression equations were found for

the non/mono-ortho and multi-ortho groups of congeners containing two to seven Cl atoms,

(i) non/mono – ortho:

$$\log K_{OA} = (-1.268) \log P_L + 6.135 \quad (R = 0.997) \quad (9a)$$

(ii) multi – ortho:

$$\log K_{OA} = (-1.015) \log P_L + 6.490 \quad (R = 0.998) \quad (9b)$$

Thus the preference to use of P_L and K_{OA} actually depends on the availability of the two parameters.

The objective of this paper is to obtain the parameters A_L and B_L for P_L and A_O and B_O for K_{OA} for all 209 PBDE congeners, which is enable us to obtain the values of P_L and K_{OA} at any temperature within the environmentally relevant temperature range.

2. Methods

2.1. Relationship between $\log P_L$ and $\log K_{OA}$

The relationship between P_L and K_{OA} can be expressed as (Finizio et al., 1997; Harner and Shoeib, 2002)

$$K_{OA} = RT/(\gamma_O V_O P_L) \quad (10a)$$

where R is the universal gas constant, T is the absolute temperature, γ_O is the activity coefficient of chemicals in octanol, and V_O is the molar volume of octanol ($157 \text{ cm}^3 \text{ mol}^{-1}$). Eq. (10a) has its logarithm form as:

$$\log K_{OA} = -\log P_L + \log(RT/(V_O \gamma_O)) \quad (10b)$$

According to Raoult's law, γ_O approaches unity for an ideal solution. It has been found that for several classes of SVOCs, including PBDEs, γ_O values fall within 1 and 10, indicating near ideal behavior due to that PBDE molecules and octanol molecules are both slightly polar (Harner and Shoeib, 2002). Thus, we calculated the values of $\log(RT/V_O \gamma_O)$ with γ_O value equal to the mean of 5, founding that they are a weak function of temperature, from 6.37 at -50°C to 6.53 at $+50^\circ\text{C}$, a rise of 0.16 due to the 100°C increase in temperature. Taking a mean value of 6.46 for $\log(RT/V_O \gamma_O)$, Eq. (10b) leads to

$$\log K_{OA} = -\log P_L + 6.46 \quad (11)$$

The simple Eq. (11) allows us to calculate the values of $\log K_{OA}$ as a function of $\log P_L$ at any temperature for any PBDE congeners and vice versa. Indeed, empirical Eqs. (8) and (9a), (9b) are very similar to Eq. (11), which can be considered as the rationality of the derived Eq. (11).

There are other ways to relate the two parameters K_{OA} and P_L too. One is the combination of the empirical Eqs. (2) and (3) (Li and Jia, 2014), which yields the following equation for PBDEs valid only in the ambient temperature range from -22 to 38°C

$$\log K_{OA} = (m_L/m_O) \log P_L + (b_L - b_O)/m_O \quad (12)$$

Using Eqs. (4) and (5a), (5b) into the above equation leads to

$$\log K_{OA} = -\log P_L + (0.081T - 20.220)/(0.011T - 2.742) \quad (13)$$

showing that, differently from Eq. (11), the relationship between $\log P_L$ and $\log K_{OA}$ in Eq. (13) is dependent on temperature.

Another simple way to get the relationship between $\log P_L$ and $\log K_{OA}$ is directly from Eqs. (6) and (7), which leads to

$$\log K_{OA} = (B_O/B_L) \log P_L + B_O (A_O/B_O - A_L/B_L) \quad (14)$$

Different from Eqs. (11) and (13), Eq. (14) indicates that the relationship between $\log P_L$ and $\log K_{OA}$ is relevant to PBDE congeners but independent of temperature. Comparing Eq. (14) with Eq. (11) leads to the relationship between A_O and B_O with A_L and B_L as

$$B_L = -B_O \quad (15a)$$

$$A_L = 6.46 - A_O \quad (15b)$$

2.2. Equations to calculate A_O and B_O

The parameters of A_O and B_O can be obtained by Wania et al. (2002)

$$B_O = \Delta U_{OA} / \ln(10) R \quad (16a)$$

$$A_O = \log K_{OA0} - B_O/T_0 \quad (16b)$$

where K_{OA0} is the value at reference temperature T_0 (for example, $298 \text{ K} = 25^\circ\text{C}$), ΔU_{OA} is the internal energy of phase transfer between octanol and air in J mol^{-1} , and R is the universal gas constant ($= 8.314 \text{ Pa m}^3 \text{ mol}^{-1} \text{ K}^{-1}$). Wania and et al. (2002) obtained the values of ΔU_{OA} for 22 PBDE congeners using relative gas chromatographic retention time (Table S4). Regression analysis of ΔU_{OA} with the mole mass (MW) for these congeners suggests that over 97% of the variability of ΔU_{OA} can be explained by MW (see Fig. S1A) with the following equation:

$$\Delta U_{OA} = 0.1056 \text{ MW} + 39.089 \quad (R^2 = 0.97) \quad (17)$$

With this equation, we are able to calculate the values of ΔU_{OA} for all 209 PBDE congeners as given in Table S4 and Fig. S1B.

2.3. Values of $\log K_{OA}$ and $\log P_L$ at 25°C

It is obvious from Eq. (16b) that the values of $\log K_{OA0}$ at 25°C (298 K) are important parameters in calculating the values of A_O . It has been reported that direct experimental measurements of these parameters for PBDEs are difficult and expensive due to extremely low water solubility and vapor pressure and the large number of congeners (Yue and Li, 2013). Thus, for those not available from experimental measurement, the quantitative structure–property relationship (QSPR) method has been used to predict their values (Dunnivant et al., 1992; Li et al., 2008; Liang et al., 1997; Mansouri et al., 2012; Papa et al., 2009; Xu et al., 2007; Yue and Li, 2013). There are three datasets of $\log K_{OA}$ and $\log P_L$ at 25°C available for all 209 PBDE congeners (Papa et al., 2009; Xu et al., 2007; Yue and Li, 2013) which are reproduced in Table S5. Relationships between $\log K_{OA}$ and $\log P_L$ at 25°C for these three datasets are presented in Fig. S2, indicating that the data by Papa et al. (2009) match Eq. (11) better than the other two. The three datasets are compared with the experimentally measured data of $\log K_{OA}$ at 25°C (Harner and Shoeib, 2002; Wania et al., 2002) presented in Fig. S3 and Table S6 with the deviations are given in Table S7. It is obvious that, the three datasets match the data by Wania et al. (2002) much better than those by Harner and Shoeib (2002), and among the three datasets, the data by Papa et al. (2009) has the least deviation of K_{OA} (to Wania et al., 2002: $-4.84\% \pm 26.48\%$ (Papa et al., 2009) vs. $10.68\% \pm 37.99\%$ (Xu et al., 2007) and $47.04\% \pm 137.43\%$ (Yue and Li, 2013); to Harner and Shoeib, 2002: $18.82\% \pm 169.29\%$ vs. $69.16\% \pm 220.52\%$ and $384.79\% \pm 944.73\%$). Thus, in the present study, the data of $\log K_{OA0}$ at 25°C from Papa et al. (2009)

Table 1
Parameters A_L , B_L , A_O , and B_O for all the 209 PBDE congeners.

PBDE	A_O	B_O	A_L	B_L
BDE-1	−4.14	3415	10.60	−3415
BDE-2	−3.90	3415	10.36	−3415
BDE-3	−3.70	3415	10.16	−3415
BDE-4	−4.93	3851	11.39	−3851
BDE-5	−4.71	3851	11.17	−3851
BDE-6	−4.71	3851	11.17	−3851
BDE-7	−4.49	3851	10.95	−3851
BDE-8	−4.49	3851	10.95	−3851
BDE-9	−4.71	3851	11.17	−3851
BDE-10	−4.95	3851	11.41	−3851
BDE-11	−4.49	3851	10.95	−3851
BDE-12	−4.26	3851	10.72	−3851
BDE-13	−4.26	3851	10.72	−3851
BDE-14	−4.49	3851	10.95	−3851
BDE-15	−4.03	3851	10.49	−3851
BDE-16	−5.51	4286	11.97	−4286
BDE-17	−5.29	4286	11.75	−4286
BDE-18	−5.51	4286	11.97	−4286
BDE-19	−5.73	4286	12.19	−4286
BDE-20	−5.29	4286	11.75	−4286
BDE-21	−5.07	4286	11.53	−4286
BDE-22	−5.06	4286	11.52	−4286
BDE-23	−5.29	4286	11.75	−4286
BDE-24	−5.51	4286	11.97	−4286
BDE-25	−5.06	4286	11.52	−4286
BDE-26	−5.29	4286	11.75	−4286
BDE-27	−5.51	4286	11.97	−4286
BDE-28	−4.84	4286	11.30	−4286
BDE-29	−5.06	4286	11.52	−4286
BDE-30	−5.28	4286	11.74	−4286
BDE-31	−5.06	4286	11.52	−4286
BDE-32	−5.29	4286	11.75	−4286
BDE-33	−5.06	4286	11.52	−4286
BDE-34	−5.29	4286	11.75	−4286
BDE-35	−4.84	4286	11.3	−4286
BDE-36	−5.06	4286	11.52	−4286
BDE-37	−4.61	4286	11.07	−4286
BDE-38	−4.84	4286	11.3	−4286
BDE-39	−4.84	4286	11.3	−4286
BDE-40	−6.08	4722	12.54	−4722
BDE-41	−5.86	4722	12.32	−4722
BDE-42	−5.86	4722	12.32	−4722
BDE-43	−6.08	4722	12.54	−4722
BDE-44	−6.08	4722	12.54	−4722
BDE-45	−6.30	4722	12.76	−4722
BDE-46	−6.30	4722	12.76	−4722
BDE-47	−5.64	4722	12.1	−4722
BDE-48	−5.86	4722	12.32	−4722
BDE-49	−5.86	4722	12.32	−4722
BDE-50	−6.08	4722	12.54	−4722
BDE-51	−6.08	4722	12.54	−4722
BDE-52	−6.08	4722	12.54	−4722
BDE-53	−6.30	4722	12.76	−4722
BDE-54	−6.52	4722	12.98	−4722
BDE-55	−5.64	4722	12.1	−4722
BDE-56	−5.64	4722	12.1	−4722
BDE-57	−5.86	4722	12.32	−4722
BDE-58	−5.86	4722	12.32	−4722
BDE-59	−6.08	4722	12.54	−4722
BDE-60	−5.41	4722	11.87	−4722
BDE-61	−5.64	4722	12.1	−4722
BDE-62	−5.86	4722	12.32	−4722
BDE-63	−5.64	4722	12.1	−4722
BDE-64	−5.86	4722	12.32	−4722
BDE-65	−6.08	4722	12.54	−4722
BDE-66	−5.42	4722	11.88	−4722
BDE-67	−5.64	4722	12.1	−4722
BDE-68	−5.64	4722	12.1	−4722
BDE-69	−5.86	4722	12.32	−4722
BDE-70	−5.64	4722	12.1	−4722
BDE-71	−5.86	4722	12.32	−4722
BDE-72	−5.86	4722	12.32	−4722
BDE-73	−6.08	4722	12.54	−4722
BDE-74	−5.41	4722	11.87	−4722
BDE-75	−5.63	4722	12.09	−4722

Table 1 (continued)

PBDE	A_O	B_O	A_L	B_L
BDE-76	−5.64	4722	12.1	−4722
BDE-77	−5.19	4722	11.65	−4722
BDE-78	−5.41	4722	11.87	−4722
BDE-79	−5.41	4722	11.87	−4722
BDE-80	−5.64	4722	12.1	−4722
BDE-81	−5.19	4722	11.65	−4722
BDE-82	−6.43	5157	12.89	−5157
BDE-83	−6.65	5157	13.11	−5157
BDE-84	−6.87	5157	13.33	−5157
BDE-85	−6.24	5157	12.7	−5157
BDE-86	−6.43	5157	12.89	−5157
BDE-87	−6.43	5157	12.89	−5157
BDE-88	−6.65	5157	13.11	−5157
BDE-89	−6.65	5157	13.11	−5157
BDE-90	−6.43	5157	12.89	−5157
BDE-91	−6.65	5157	13.11	−5157
BDE-92	−6.65	5157	13.11	−5157
BDE-93	−6.87	5157	13.33	−5157
BDE-94	−6.87	5157	13.33	−5157
BDE-95	−6.87	5157	13.33	−5157
BDE-96	−7.10	5157	13.56	−5157
BDE-97	−6.43	5157	12.89	−5157
BDE-98	−6.65	5157	13.11	−5157
BDE-99	−6.21	5157	12.67	−5157
BDE-100	−6.44	5157	12.9	−5157
BDE-101	−6.43	5157	12.89	−5157
BDE-102	−6.65	5157	13.11	−5157
BDE-103	−6.65	5157	13.11	−5157
BDE-104	−6.87	5157	13.33	−5157
BDE-105	−5.99	5157	12.45	−5157
BDE-106	−6.21	5157	12.67	−5157
BDE-107	−6.21	5157	12.67	−5157
BDE-108	−6.21	5157	12.67	−5157
BDE-109	−6.43	5157	12.89	−5157
BDE-110	−6.43	5157	12.89	−5157
BDE-111	−6.43	5157	12.89	−5157
BDE-112	−6.65	5157	13.11	−5157
BDE-113	−6.65	5157	13.11	−5157
BDE-114	−5.99	5157	12.45	−5157
BDE-115	−6.21	5157	12.67	−5157
BDE-116	−6.43	5157	12.89	−5157
BDE-117	−6.43	5157	12.89	−5157
BDE-118	−5.99	5157	12.45	−5157
BDE-119	−6.21	5157	12.67	−5157
BDE-120	−6.21	5157	12.67	−5157
BDE-121	−6.43	5157	12.89	−5157
BDE-122	−6.21	5157	12.67	−5157
BDE-123	−5.99	5157	12.45	−5157
BDE-124	−6.21	5157	12.67	−5157
BDE-125	−6.43	5157	12.89	−5157
BDE-126	−5.80	5157	12.26	−5157
BDE-127	−5.99	5157	12.45	−5157
BDE-128	−6.78	5592	13.24	−5592
BDE-129	−7.00	5592	13.46	−5592
BDE-130	−7.00	5592	13.46	−5592
BDE-131	−7.22	5592	13.68	−5592
BDE-132	−7.22	5592	13.68	−5592
BDE-133	−7.22	5592	13.68	−5592
BDE-134	−7.45	5592	13.91	−5592
BDE-135	−7.45	5592	13.91	−5592
BDE-136	−7.67	5592	14.13	−5592
BDE-137	−6.78	5592	13.24	−5592
BDE-138	−6.78	5592	13.24	−5592
BDE-139	−7.00	5592	13.46	−5592
BDE-140	−7.00	5592	13.46	−5592
BDE-141	−7.00	5592	13.46	−5592
BDE-142	−7.22	5592	13.68	−5592
BDE-143	−7.22	5592	13.68	−5592
BDE-144	−7.22	5592	13.68	−5592
BDE-145	−7.45	5592	13.91	−5592
BDE-146	−7.00	5592	13.46	−5592
BDE-147	−7.22	5592	13.68	−5592
BDE-148	−7.22	5592	13.68	−5592
BDE-149	−7.22	5592	13.68	−5592
BDE-150	−7.45	5592	13.91	−5592
BDE-151	−7.45	5592	13.91	−5592

Table 1 (continued)

PBDE	A _O	B _O	A _L	B _L
BDE-152	-7.67	5592	14.13	-5592
BDE-153	-6.76	5592	13.22	-5592
BDE-154	-7.02	5592	13.48	-5592
BDE-155	-7.22	5592	13.68	-5592
BDE-156	-6.53	5592	12.99	-5592
BDE-157	-6.56	5592	13.02	-5592
BDE-158	-6.78	5592	13.24	-5592
BDE-159	-6.78	5592	13.24	-5592
BDE-160	-7.00	5592	13.46	-5592
BDE-161	-7.00	5592	13.46	-5592
BDE-162	-6.78	5592	13.24	-5592
BDE-163	-7.00	5592	13.46	-5592
BDE-164	-7.00	5592	13.46	-5592
BDE-165	-7.22	5592	13.68	-5592
BDE-166	-6.78	5592	13.24	-5592
BDE-167	-6.56	5592	13.02	-5592
BDE-168	-6.78	5592	13.24	-5592
BDE-169	-6.34	5592	12.8	-5592
BDE-170	-7.35	6027	13.81	-6027
BDE-171	-7.57	6027	14.03	-6027
BDE-172	-7.57	6027	14.03	-6027
BDE-173	-7.80	6027	14.26	-6027
BDE-174	-7.80	6027	14.26	-6027
BDE-175	-7.80	6027	14.26	-6027
BDE-176	-8.02	6027	14.48	-6027
BDE-177	-7.80	6027	14.26	-6027
BDE-178	-8.02	6027	14.48	-6027
BDE-179	-8.24	6027	14.7	-6027
BDE-180	-7.35	6027	13.81	-6027
BDE-181	-7.57	6027	14.03	-6027
BDE-182	-7.57	6027	14.03	-6027
BDE-183	-7.44	6027	13.9	-6027
BDE-184	-7.80	6027	14.26	-6027
BDE-185	-7.80	6027	14.26	-6027
BDE-186	-8.02	6027	14.48	-6027
BDE-187	-7.80	6027	14.26	-6027
BDE-188	-8.02	6027	14.48	-6027
BDE-189	-7.13	6027	13.59	-6027
BDE-190	-7.35	6027	13.81	-6027
BDE-191	-7.35	6027	13.81	-6027
BDE-192	-7.57	6027	14.03	-6027
BDE-193	-7.57	6027	14.03	-6027
BDE-194	-7.93	6463	14.39	-6463
BDE-195	-8.15	6463	14.61	-6463
BDE-196	-8.15	6463	14.61	-6463
BDE-197	-8.37	6463	14.83	-6463
BDE-198	-8.37	6463	14.83	-6463
BDE-199	-8.37	6463	14.83	-6463
BDE-200	-8.59	6463	15.05	-6463
BDE-201	-8.59	6463	15.05	-6463
BDE-202	-8.81	6463	15.27	-6463
BDE-203	-8.15	6463	14.61	-6463
BDE-204	-8.37	6463	14.83	-6463
BDE-205	-7.93	6463	14.39	-6463
BDE-206	-8.72	6898	15.18	-6898
BDE-207	-8.94	6898	15.4	-6898
BDE-208	-9.16	6898	15.62	-6898
BDE-209	-9.50	7333	15.96	-7333

were used to calculate the values of A_O using Eq. (16b). Note that the deviations are based on K_{OA0} rather than $\log K_{OA0}$. As an example, for BDE-28, the deviation of K_{OA0} from data by Papa et al. (2009) to that by Harner and Shoeib (2002) (see Table S6) is calculated as $(10^{9.54} - 10^{9.51}) / 10^{9.51} = 7.07\%$ (see Table S7).

3. Results

3.1. Values of A_O & B_O and A_L & B_L

Sorting out the whole process described in the previous sections, we calculated the values of Clausius-Clapeyron parameter A_O & B_O and A_L & B_L for all 209 PBDE congeners at the following steps. First, a regression

analysis of the experimentally measured internal energy ΔU_{OA} for 22 PBDE congeners (Wania and et al., 2002) led to the values of ΔU_{OA} for all 209 PBDE congeners (Table S4). Next, B_O was computed using the values of ΔU_{OA} and Eq. (16a). Third, using the values of B_O and the values of $\log K_{OA0}$ at 25 °C (Papa et al., 2009) (see Table S5), we calculated the values of A_O from Eq. (16b). Finally, the values of the parameter A_L and B_L are obtained using Eqs. (15a), (15b) for all 209 PBDE congeners. The calculated the parameter A_L , B_L , A_O , and B_O for all 209 PBDE congeners are presented in Table 1.

By using the values of A_O and B_O , $\log K_{OA}$ at any ambient air temperature can be obtained for all 209 PBDE congeners using Eq. (7). Similarly, using the values of A_L and B_L , $\log P_L$ at any ambient air temperature can be calculated by using Eq. (6). These two sets of the values of $\log K_{OA}$ and $\log P_L$ satisfy Eq. (11).

3.2. Comparison of A_L , B_L , A_O , and B_O between the present study and other sources

To evaluate the values of A_L , B_L , A_O , and B_O listed in Table 1, these data are compared to those available from other sources for some selected PBDE congeners (Tittlemier et al., 2002; Wong et al., 2001; Harner and Shoeib, 2002) and the results are presented in Table S8 for A_L and B_L and Table S9 for A_O and B_O . Table S8 shows that data of A_L and B_L from our study are in a great agreement with those given by Wong et al. (2001) with the deviation of $-3.64\% \pm 3.51\%$ for A_L and $-2.05\% \pm 2.35\%$ for B_L and those given by Tittlemier et al. (2002) with the deviation of $3.83\% \pm 10.88\%$ for A_L and $-1.61\% \pm 12.17\%$ for B_L (Table S8b); Table S9 indicates that, in comparison with the data given by Harner and Shoeib (2002), a great consistence was found for B_O with the deviation of $2.91\% \pm 12.68\%$, but a higher difference for A_O with the deviation of $19.29\% \pm 39.07\%$, as shown in Table S9b. The major reason for this higher inconsistency of A_O is possibly due to the discrepancies of the values of $\log K_{OA}$ at 25 °C between those from Papa data set (Papa et al., 2009) used in this study and the experimental measured data by Harner and Shoeib (2002) (see Sections 2.3 and 3.1).

It is also interesting to note the variations of A_L , $|B_L|$, $|A_O|$, and B_O from this study and other sources vs. the mole mass (MW) of PBDE congeners depicted in Fig. S4, which indicates that the values of A_L and the absolute values of B_L from the present study and those by Wong et al. (2001) and Tittlemier et al. (2002) are strongly correlated with MW for selected PBDE congeners (the range of correlation coefficient R is from 0.94 to 1.00). However, while the absolute values of A_O and the values of B_O from the present study are strongly correlated with the MW for selected PBDE congeners (R equals to 0.98 for $|A_O|$ and 1.00 for B_O), those from Harner and Shoeib (2002) are not, with correlation data of 0.02 for $|A_O|$ and 0.41 for B_O .

3.3. $\log P_L$ and $\log K_{OA}$ as functions of temperature

Since the application of coefficients A_O & B_O and A_L & B_L is to calculate $\log K_{OA}$ and $\log P_L$, respectively, it could be better to evaluate the values of K_{OA} and P_L predicted using these parameters (A_O & B_O and A_L & B_L) determined in this study with the data of K_{OA} and P_L predicted by other groups.

By using Eq. (6), we calculated $\log P_L$ at different ambient temperature using the parameters A_L and B_L taken from the present study and the other sources (Table S6), and the results are depicted in Fig. 1 for BDE-47, -66, -77, -99, -153, and -190 at temperatures ranged -30 – 30 °C, indicating that the results from the present study are consistent with those by Wong et al. (2001) and Tittlemier et al. (2002), especially to the latter. The boundaries of ± 0.3 log unit for $\log P_L$ (equivalent to a factor of 2 for P_L) are also shown, suggesting the difference of P_L between our data and the published data by Wong et al. (2001) and Tittlemier et al. (2002) are within or almost within 2 factor of magnitude.

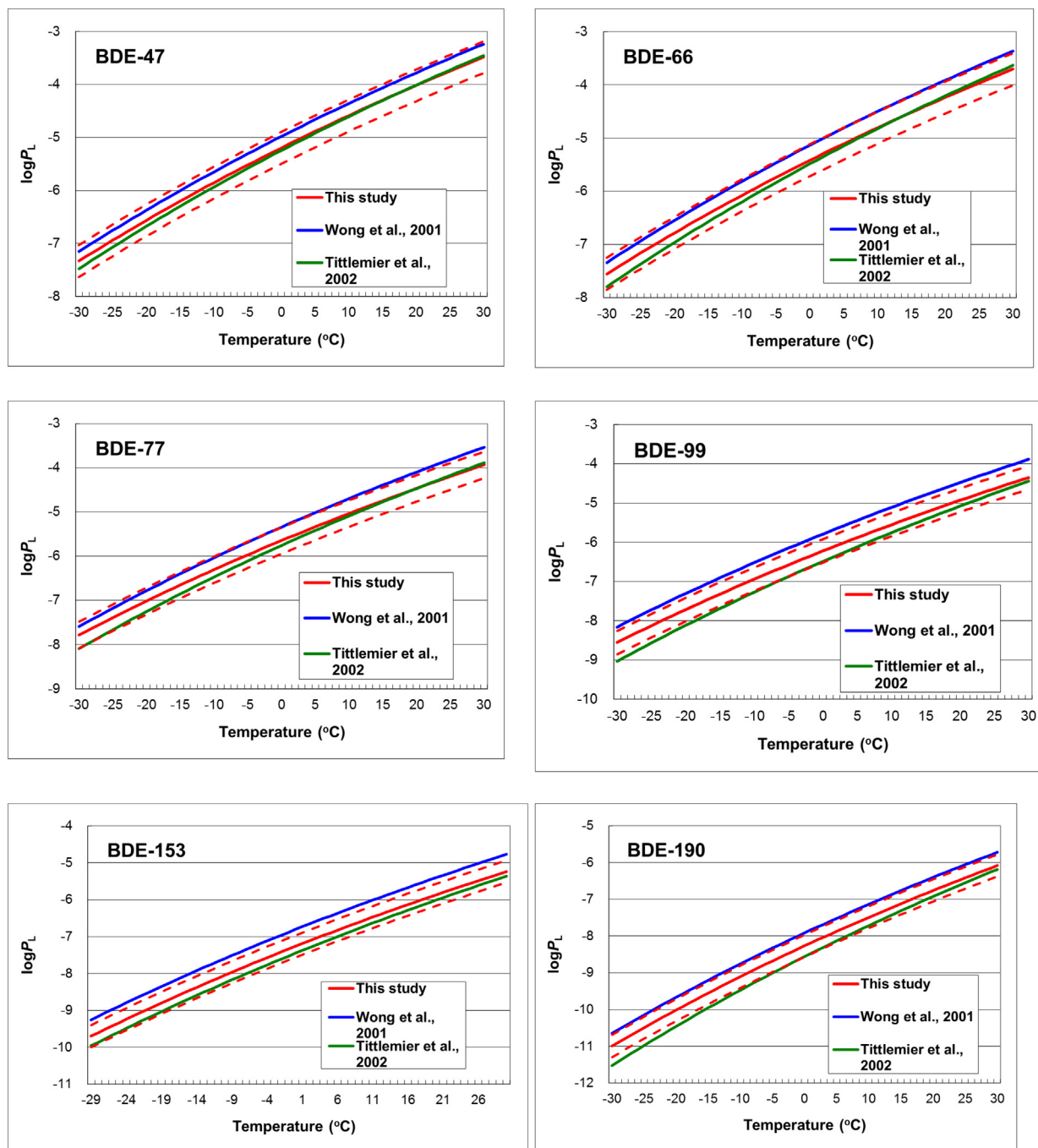


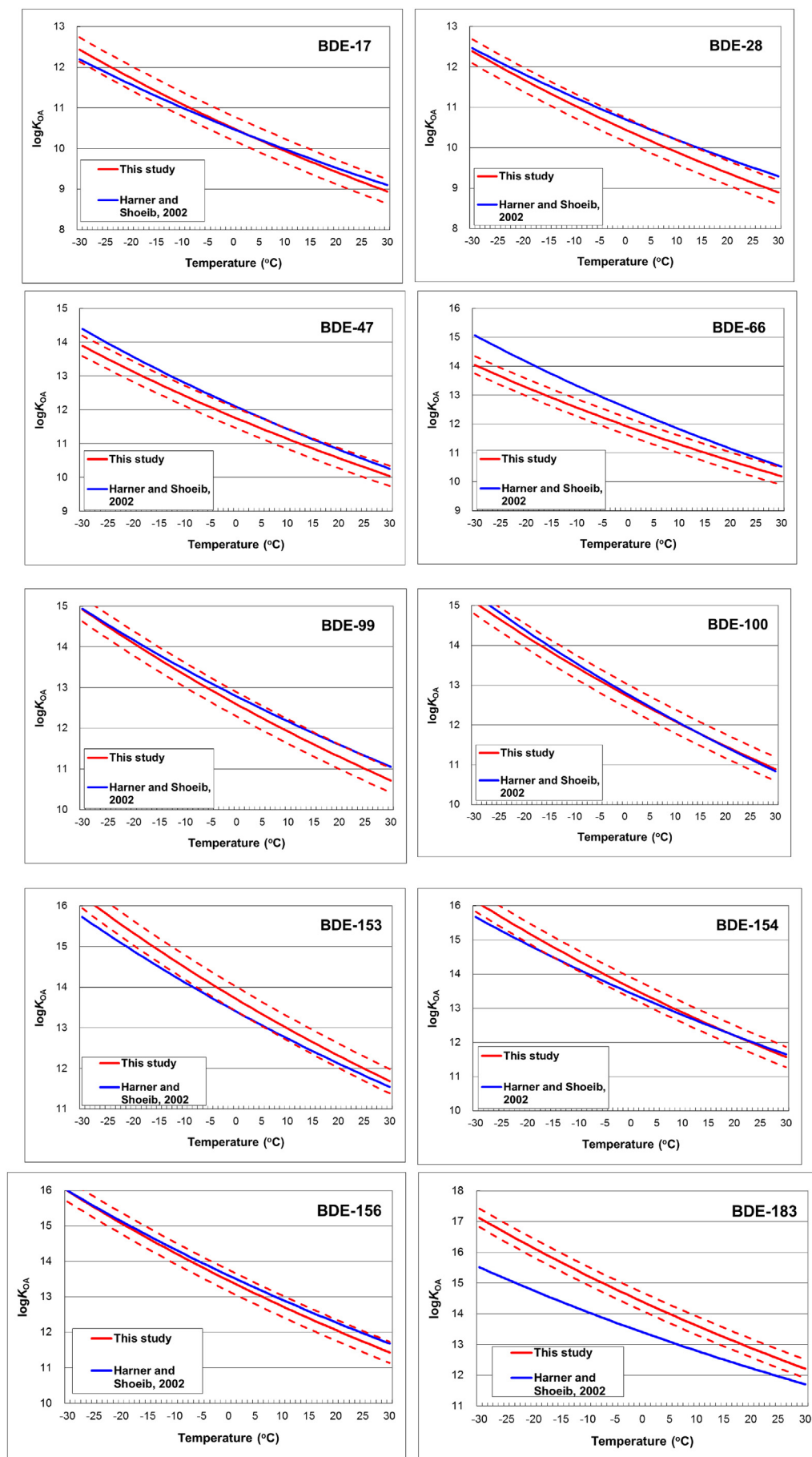
Fig. 1. Comparison of our results of $\log P_L$ at ambient temperature range of $-30 - 30^\circ\text{C}$ for BDE-47, -66, -77, -99, -153, and -190 to the values reported by previous literature (Tittlemier et al., 2002; Wong et al., 2001). The two dashed red lines give the ± 0.3 (log unit for $\log P_L$, equivalent to 2 factor of P_L) of the red line produced in this study. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

To illuminate this temperature effect on $\log P_L$, the values of $\log P_L$ for BDE-47 is -7.33 at -30°C and -3.48 at 30°C , corresponding to a difference >7000 -fold increase in P_L over this 60°C rise in temperature, while for BDE-190, this increase is much higher, $>80,000$ times over the same temperature range, with the values of $\log P_L$ from -10.99 at -30°C to -6.08 at 30°C .

By using Eq. (6), we calculated $\log K_{OA}$ for selected PBDE congeners at the temperature ranged from -30 to 30°C using the parameters A_O

and B_O taken from the present study and those by Harner and Shoeib (2002) (Table S9a), and the results are presented in Fig. 2. Obvious deviations are observed for the data of A_O from our study to those given by Harner and Shoeib (2002) as shown in Table S9b. However, as shown in Fig. 2, the values of $\log K_{OA}$ calculated using the values of A_O and B_O from our study match the data from Harner and Shoeib (2002) well in general within ~ 2 factor of magnitude, with 2 exceptions of BDE-66 and -183. The worst is for BDE-183, which is not unexpected. As pointed

Fig. 2. Comparison of our results of $\log K_{OA}$ obtained using Eq. (12) at the temperature ranged from -30 to 30°C for 12 PBDE congeners from our study and the study by Harner and Shoeib (2002). The two dashed red lines give the ± 0.3 (log unit for $\log P_L$, equivalent to 2 factor of P_L) of the red line produced in this study. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)



out previously (Wong et al., 2001; Xiao and Wania, 2003), the reported K_{OA} values for BDE-183 (Harner and Shoeib, 2002) tend to be too low. This suggests that the parameters A_O and B_O determined in this study are capable to predict K_{OA} values within the environmental temperature range despite the relatively high discrepancies in the reported A_O values for some congeners.

To elaborate on this temperature effect on $\log K_{OA}$, according to our calculation, $\log K_{OA}$ for BDE-17 is 12.44 at -30°C and 8.95 at 30°C , corresponding to a difference >3000-fold decrease in K_{OA} over this 60°C rise in temperature, while for BDE-183, this decrease in K_{OA} is much greater, becoming >80,000 times over the same temperature range, with the values of $\log K_{OA}$ from 17.12 at -30°C to 12.21 at 30°C .

3.4. Data for BDE-209

G/P partition behavior of BDE-209 has become special focus point in the recent years due to its high value of K_{OA} and low value of P_L (Bogdal et al., 2014; Breivik et al., 2006; Li et al., 2017; Li et al., 2015). The values for $\log K_{OA}$ for BDE-209, however, are lacking and only the value at 25°C has been estimated from different groups: 15.27 by Wania and Dugani (2003), 14.98 by Cetin and Odabasi (2008), 16.8 by Schenker et al. (2008), and 15.24 by Zhang et al. (2012). In our previous work (Li et al., 2017) we estimate the values of $\log K_{OA}$ for BDE-209 as a function of temperature using the $\log K_{OA0}$ value of 15.27 (Wania and Dugani, 2003) and the ΔU_{OA} value of $80,000\text{ J}\cdot\text{mol}^{-1}$ (Breivik et al., 2006) in Eqs. (16a), (16b), and calculated values of A_O and B_O for BDE-209, which are 1.25 and 4179, respectively (Li et al., 2017), leading to the values of $\log K_{OA}$ from 14.2 at $+50^\circ\text{C}$ to 20.0 at -50°C . The value of ΔU_{OA} calculated in the present study is $140,400\text{ J}\cdot\text{mol}^{-1}$ (Table S5), thus the Clausius-Clapeyron parameter are -9.50 for A_O and 7333 for B_O , leading the values of $\log K_{OA}$ from 13.20 at $+50^\circ\text{C}$ to 23.38 at -50°C (see Fig. S5A). Although the values of $\log K_{OA}$ are different from these two studies, both these two datasets of $\log K_{OA}$ data indicate the same results, which is that BDE-209 is within the maximum partitioning (MP) domain over the entire environmentally relevant temperature range of -50°C to $+50^\circ\text{C}$ (Li et al., 2017). The values of $\log P_L$ for BDE-209 as a function of temperature from the present study are also depicted in Fig. S5B, showing the values of $\log P_L$ for BDE-209 from -6.74 at $+50^\circ\text{C}$ to -16.92 at -50°C .

4. Discussions and implication

4.1. Uncertainty

Recapitulating the essential points to calculate the values of Clausius-Clapeyron parameter A_O & B_O and A_L & B_L for all 209 PBDE congeners listed in Table 1, there are three crucial elements used in the process: the data of $\log K_{OA0}$ at 25°C , Eqs. (16a), (16b) used to calculate A_O and B_O , and Eqs. (15a), (15b) to calculate A_L & B_L . As explained in Section 2.3, the data of $\log K_{OA0}$ at 25°C from Papa et al. (2009) used in the present study is the best dataset match the experimentally measured data both by Harner and Shoeib (2002) and Wania et al. (2002); Eqs. (16a), (16b) used to calculate A_O and B_O was suggested and used by Wania et al. (2002) in their study, and considered as a useful method in predicting the values of $\log K_{OA}$. Eqs. (15a), (15b) was first suggested and applied to calculate A_L & B_L in the present study. As described in Section 3.2, A_L and B_L obtained from Eqs. (15a), (15b) and also $\log P_L$ calculated from these two parameters are in great consistent with those given by Wong et al. (2001) and Tittlemier et al. (2002).

To evaluate the accuracy of the data produced in this study (Table 1), we further check the data of P_L at the temperature of 25°C calculated in the present study (Table S5) with experimentally measured data by Wong et al. (2001) and Tittlemier et al. (2002). The results presented in Table S10 suggest reasonable estimation accuracy, with a stand deviation of $29.94\% \pm 35.09\%$ for Wong et al. (2001) and

a stand deviation of $28.07\% \pm 74.61\%$ for Tittlemier et al. (2002). Note that the deviations are based on P_L rather than $\log P_L$. As an example, for BDE-28, the deviation of P_L from our study to that by Wong et al. (2001) is calculated as $(10^{-3.08} - 10^{-2.65}) / 10^{-2.65} = -62.61\%$ (Table S10).

Beyer et al. (2002) suggested five levels for uncertainty factor ranging from 0 (high accuracy) to 5 (highly uncertain) assigned to physico-chemical property for SVOCs, which is based on judgment and subjective (Yue and Li, 2013). Followed by Yue and Li (2013), we assign conservatively an uncertainty factor of 1 for the dataset of A_L and B_L but 2 for the dataset of A_O and B_O listed in Table 1. As stated by Wong et al. (2001), for very low volatility compounds, being within a factor of 2 of a literature value is well within the precision of the classical techniques. Indeed, even for direct measurement of K_{OA} , deviations resulted from repeated measurements of K_{OA} of the same compound by the same research group could be on a factor of 1.6 (0.2 Log units) (Wania et al., 2002).

In light of these inherent uncertainties described above, the obviously observed agreement between data presented in Table 1 and those published is very good, which suggests that the dataset produced in this study can be served to estimate both the $\log K_{OA}$ and $\log P_L$ of all 209 PBDE congeners at all ambient temperature.

4.2. Other methods to link $\log K_{OA}$ and $\log P_L$

There are other ways to link $\log K_{OA}$ and $\log P_L$ as described by Eqs. (13) and (14). It is interesting to compare these two equations with Eq. (11). The sum of $\log P_L$ and $\log K_{OA}$ is a constant (6.46) from Eq. (11), but a function of temperature $((0.081T - 20.220) / (0.011T - 2.742))$ from Eq. (13) and PBDE congener dependent (a function of Clausius-Clapeyron parameter), and independent of temperature from Eq. (14). Fig. S6 presents the comparison of $\log P_L$ plus $\log K_{OA}$ between Eqs. (11) and (13), showing a reasonable consistence between these two equations. It should be pointed out that, Eq. (14) is valid only in the temperature range between -22°C to 38°C . The comparison between Eqs. (11) and (14) for 10 different PBDE congeners (BDE-28, 47, 66, 77, 85, 99, 100, 153, 154, and 183) is depicted in Fig. S7. It is clear that, for all these 10 PBDE congeners, the values of $\log K_{OA}$ and $\log P_L$ from Eq. (11) are presented by one straight line (the red one), while the results by Eq. (14) by 10 lines for the 10 PBDE congeners, separately, all closely surrounding the red line. The lower of the value of $\log P_L$, the greater of the departure of the values given by Eq. (14) from the line of Eq. (11) becomes. Once again, the greatest departure is for BDE-183.

It is obvious that Eq. (11) is better than Eqs. (13) and (14) not only because of its simple form and its independence on congeners and ambient temperatures, but its theoretical background as well.

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Conflict of interest

There is no conflict of interest among all the authors.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.scitotenv.2018.02.054>.

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