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# Melting points and enthalpies of fusion of anthracene and its heteroatomic counterparts

**Jillian L. Goldfarb · Indrek Külaots**

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**Abstract** Anthracene is a common byproduct of incomplete combustion of fossil fuels and other anthropogenic sources. Its heteroatomic counterparts, including 9-bromoanthracene, 1,5-dibromoanthracene, 9,10-dibromoanthracene, 2-chloroanthracene, 9,10-dichloroanthracene, 9-anthraldehyde, 2-anthracenecarboxylic acid, 9-anthracenecarboxylic acid, and anthraquinone, are formed through various mechanistic pathways during the combustion process. We use a differential scanning calorimeter to measure the melting points and enthalpies of fusion of these compounds. As expected, we find no correlation between molecular mass and melting point and enthalpy of fusion—rather the type, number and position of the heteroatoms substituted on the parent molecule all influence its fusion thermodynamics. A wide range of melting points is noted for the same substituents(s) at different carbon positions. This suggests that intermolecular forces, such as hydrogen bonding and steric repulsion, are significantly impacted by the position of the substituents on the linear anthracene parent molecular. In addition, different substituents at the same position further suggest that the electronegativity/polarity of a given atom strongly influences the observed fusion behavior.

**Keywords** Anthracene · Heteroatom · PAC · Polycyclic aromatic compound · Melting point · Enthalpy of fusion

## Introduction

Polycyclic aromatic compounds (PAC) are a frequently encountered class of environmental pollutants resulting, on a large scale, from the incomplete combustion of fossil fuels and other anthropogenic sources. Anthracene, a PAC composed of three fused benzene rings, is routinely found at former manufactured gas plant sites and resides on the EPA's Priority Pollutant List of compounds for its carcinogenic nature and ubiquitous positioning in the environment. During an inquiry into the thermodynamics of these compounds, we encountered a distinct lack of melting points and fusion enthalpies for many PAC. Peters et al. [1] also note this shortage of fusion enthalpies for PAC in the literature; this dearth of data may hamper environmental models and risk assessments. In this investigation, we examine the fusion thermodynamics of anthracene and some of its heteroatom-containing counterparts, including those with halogen and oxygen substituents, and compare their melting points to those of compounds with similar substituents on different carbon atoms.

Polycyclic aromatic hydrocarbons (PAH), those PAC without heteroatomic substituents, may undergo a variety of halogenation mechanisms to yield PAC in various processes. Hu et al. [2] show that the presence of bromine ions significantly increases the rate of chlorination of pyrene, while simultaneously producing brominated pyrenes. The promotion of soot formation in flames by chlorine and chlorinated hydrocarbons is linked to PAH formation, as PAH are believed to be soot precursors [3]. In the presence of bromine and chlorine, it may be possible to accelerate the formation of halogenated and non-halogenated PAH [2]. PAH and oxygenated polycyclic aromatic hydrocarbons (OPAH) were shown by Rogge et al. to account for between 3.1 and 8.6% of the total identifiable fine organic

J. L. Goldfarb (✉) · I. Külaots
Division of Engineering, Brown University, 182 Hope Street, Providence, RI 02912, USA
e-mail: JillianLGoldfarb@gmail.com

I. Külaots
e-mail: Indrek_Kulaots@brown.edu

particulate matter emitted from the burning of no. 2 distillate fuel oil in an industrial scale boiler [4]. OPAH can form through the photooxidation of PAH via several mechanistic pathways [5].

Polycyclic aromatic compounds (PAC) can crystallize in five structural ways: $\beta$, $\gamma$, herringbone, sandwich herringbone, and flat sandwich herringbone, of which herringbone is the most common for elongated, unsubstituted aromatics, such as anthracene [6]. The structural arrangement of a given molecule depends on the strength of the carbon–carbon and carbon–hydrogen interactions, and the number and position of such carbon and hydrogen atoms in the molecule. In the herringbone arrangement, non-bonded carbons interact with non-parallel nearest neighbor molecules to achieve molecular stabilization through carbon–hydrogen interactions [7]. Herringbone structures are stabilized by van der Waals forces [8]. However, it is not molecular packing alone that determines melting point; anthracene melts around 490 K and phenanthrene around 373 K, although both compounds adopt a herringbone structure. Likewise, chrysene and triphenylene, with the same molecular mass (228.29 g/mol) and herringbone packing have substantially different melting points. Chrysene melts at 528 K and triphenylene at around 471 K [7]. From these literature examples and our data, we see that the melting point of a given compound is a function not only of molecular mass and molecular packing but also of intermolecular forces subtly related to the electronegativity/polarity, steric effects, and possible hydrogen bonding.

The contribution of molecular electronegativity/polarity to the melting point is well-known. The presence of heteroatoms in the molecules may decrease the melting point, as seen for 9-bromoanthracene, due to steric effects. Furthermore, widely varying effects exist for the same substituents at different carbon atom positions; 1-chloroanthracene shows a much lower melting point (627.9–630.9 K) compared to 2-chloroanthracene (768.9 K). Yet, the oxygen-containing PAC, e.g., the anthracenecarboxylic acids, usually show a higher melting point than the parent unsubstituted PAH, attributable to hydrogen bonding.

## Experimental

A Thermal Analysis (TA) Instruments 2910 Differential Scanning Calorimeter (DSC) was used to measure the melting points and heats of fusion of each compound. The cell baseline (heat flow) was calibrated at a heating rate of 5 K min$^{-1}$ in a constant, metered nitrogen flow of 50 cc min$^{-1}$. The sample cell temperature sensor was calibrated with pure indium metal (provided by Instrument Specialists, Inc.) of known melting point using hermetically sealed aluminum sample pans [9, 10]. Samples were run in the same pans (a new pan for each run) at the same heating rate and nitrogen flow as the calibration runs. Approximately 1.5–3.5 mg of sample was placed into each pan, measured using a microbalance accurate to $5 \times 10^{-4}$ mg. The PAC were obtained from TCI America, Inc. at minimum purities of 95%, as detailed in Table 1. Compounds with minimum purities below 98% (9-anthracenecarboxylic acid, at a minimum purity of 97%, 9-bromoanthracene, at a minimum purity of 95%, and 9, 10-dichloroanthracene, at a minimum purity of 96%) were purified via fractional sublimation to remove volatile impurities; this method has been shown to yield samples with purities of greater than 99% using both in-stream mass spectrometer analysis as well as gas chromatography/mass spectrometry analysis of the purified compound [11, 12]. Melting point determinations of anthraquinone (minimum purity 98%) before and after fractional sublimation yielded the same melting point (within 0.1 K). Measured melting points of other compounds of greater than 98% purity are consistent with available literature data and show reproducible experimental results, indicating there are no issues with volatile impurities.

## Results and discussion

Table 1 gives the average values obtained for each compound compared to literature values, when available. The 95% confidence intervals reported in Table 1 were calculated for each compound using KaleidaGraph's statistics function. Each compound was tested at least three times in separate sample pans to ensure reproducibility. Figure 1 shows the DSC results for two trials of anthraquinone and 9-anthraldehyde, demonstrating the high degree of reproducibility we achieved with our experiments in terms of melting point temperature and enthalpy (at least three trials for each compound were reproduced in the same manner, two are shown here for visual clarity). Of the 10 compounds measured, anthraquinone, with double-bonded oxygen atoms on the C9 and C10, had the highest melting point, though the highest enthalpy of fusion was seen for 2-anthracenecarboxylic acid. There is no correlation between molecular mass and enthalpy of fusion for these compounds. We note this thermodynamic trend among sublimation studies; many remark that the vapor pressures of these compounds cannot be predicted by molecular mass alone, as exemplified by Coutsikos et al. [13], who used a group contribution method to account for molecular structure of a given polycyclic aromatic hydrocarbon.

Tables 2 and 3 compare the effects of a given substituent and its carbon position on anthracene to the parent

**Table 1** Experimental and literature fusion data for anthracene and its heteroatomic counterparts

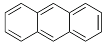
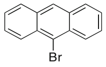
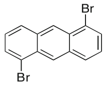
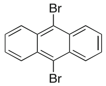
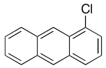
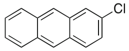
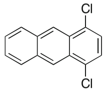
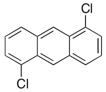
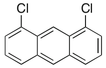
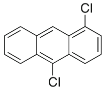
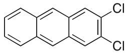
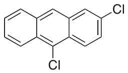
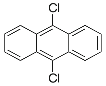
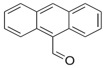
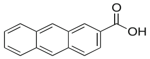
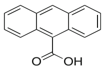
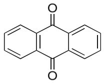
| Compound | CAS Reg. No. | Molecular weight/ g mol$^{-1}$ | Min. purity/% | Melting point/ K | Enthalpy of fusion/kJ mol$^{-1}$ | Enthalpy of sublimation/ kJ mol$^{-1}$ [11, 15, 18] | Molecular structure |
|---|---|---|---|---|---|---|---|
| Anthracene $C_{14}H_{10}$ | 120-12-7 | 178.2 | | | | |  |
| [19] | | | 99.8 | 485.9 | | | |
| [20][a] | | | | 489.7 | 28.8 | | |
| This Study | | | 99 | 489.7 ± 0.5* | 28.2 ± 0.01 | 98.5 ± 3.3 | |
| [21] | | | | 489.8 | | | |
| [22] | | | | 489.7–490.4 | | | |
| [23][a] | | | | 490.1–490.5 | | | |
| [24] | | | 99.5 | 491.2 | | | |
| [25][a] | | | | | 29.37 | | |
| 9-Bromoanthracene $C_{14}H_9Br$ | 1564-64-3 | 257.1 | | | | |  |
| [26] | | | | 373.2–374.2 | | | |
| This Study | | | 95 | 375.9 ± 1.0 | 19.2 ± 0.9 | 100.5 ± 1.8 | |
| 1,5-Dibromoanthracene $C_{14}H_8Br_2$ | 3278-82-8 | 336.0 | | | | |  |
| [27] | | | | 480.2–482.2 | | | |
| This Study | | | 98 | 482.4 ± 1.0 | 32.1 ± 1.4 | 116.7 ± 3.0 | |
| 9,10-Dibromoanthracene $C_{14}H_8Br_2$ | 523-27-3 | 336.0 | | | | |  |
| [28] | | | | 494.2–499.4 | | | |
| [29] | | | | 492.2–493.2 | | | |
| This Study | | | 98 | 497.9 ± 0.9 | 27.0 ± 0.2 | 114.2 ± 2.8 | |
| 1-Chloroanthracene $C_{14}H_9Cl$ | | 212.7 | | | | |  |
| [14] | | | | 357.7 | | | |
| 2-Chloroanthracene $C_{14}H_9Cl$ | 17135-78-3 | 212.7 | | | | |  |
| This Study | | | >98 | 495.7 ± 0.4 | 27.2 ± 1.6 | 99.3 ± 2.7 | |
| 1,4-Dichloroanthracene $C_{14}H_9Cl_2$ | | 247.1 | | | | |  |
| [17] | | | | 453.2 | | | |
| [14] | | | | 452.2–454.2 | | | |
| 1,5-Dichloroanthracene $C_{14}H_9Cl_2$ | | 247.1 | | | | |  |
| [14] | | | | 454.2–453.2 | | | |
| 1,8-Dichloroanthracene $C_{14}H_9Cl_2$ | | 247.1 | | | | |  |
| [14] | | | | 424.2–426.2 | | | |

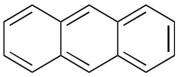
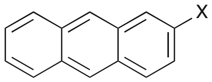
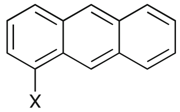
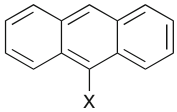
**Table 1** continued

| Compound | CAS Reg. No. | Molecular weight/ g mol$^{-1}$ | Min. purity/% | Melting point/ K | Enthalpy of fusion/kJ mol$^{-1}$ | Enthalpy of sublimation/ kJ mol$^{-1}$ [11, 15, 18] | Molecular structure |
|---|---|---|---|---|---|---|---|
| 1,10-Dichloroanthracene $C_{14}H_9Cl_2$ | | 247.1 | | | | |  |
| [14] | | | | 399.2–400.2 | | | |
| 2,3-Dichloroanthracene $C_{14}H_9Cl_2$ | | 247.1 | | | | |  |
| [17] | | | | 534.2 | | | |
| [14] | | | | 538.2–538.7 | | | |
| 2,10-Dichloroanthracene $C_{14}H_9Cl_2$ | | 247.1 | | | | |  |
| [14] | | | | 388.2–389.2 | | | |
| 9,10-Dichloroanthracene $C_{14}H_9Cl_2$ | 605-48-1 | 247.1 | | | | |  |
| [14] | | | | 483.2 | | | |
| This Study | | | >96 | 485.0 ± 0.5 | 27.4 ± 0.1 | 113.9 ± 4.9 | |
| 9-Anthraldehyde $C_{15}H_{10}O$ | 642-31-9 | 206.2 | | | | |  |
| This Study | | | >99 | 379.4 ± 0.1 | 17.9 ± 0.02 | 100.6 ± 3.9 | |
| 2-Anthracenecarboxylic acid $C_{15}H_{10}O_2$ | 613-08-1 | 222.2 | | | | |  |
| This Study | | | >98 | 559.1 ± 0.4 | 36.9 ± 1.2 | 134.8 ± 3.4 | |
| 9-Anthracenecarboxylic acid $C_{15}H_{10}O_2$ | 723-62-6 | 222.2 | | | | |  |
| This Study | | | >97 | 495.6 ± 1.0 | 34.7 ± 0.3 | 120.1 ± 3.8 | |
| Anthraquinone $C_{14}H_8O_2$ | 84-65-1 | 208.2 | | | | |  |
| [20][a] | | | | 555.2 | 32.55 | | |
| This Study | | | >98 | 558.7 ± 0.1 | 33.2 ± 0.3 | 115.5 ± 5.0 | |

[a] Data from adiabatic calorimetry measurements; experimental methods not noted in other literature cited

* 95% Confidence interval calculated as twice standard deviation

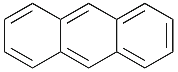
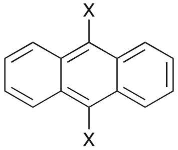
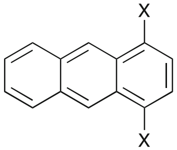
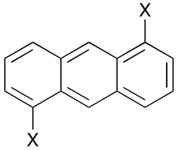
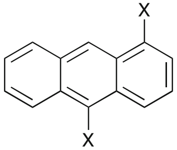
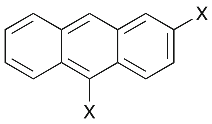
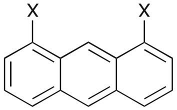
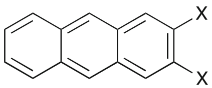
**Table 2** Single heteroatom substitution effects of -Cl, -Br and -COOH on anthracene

| | | | |
|---|---|---|---|
| Anthracene melting point/K | | | 489.7 |
| Anthracene enthalpy of fusion/kJ mol$^{-1}$ | | | 28.2 |
|  | <br>Case 1 | <br>Case 2 | <br>Case 3 |
| Substituent (X = Cl) | | | |
| Melting point (average)/K: | 495.7 | 356.2 | |
| $\Delta$MP$_{\text{(substituted-anthracene)}}$/K | 6.0 | −133.5 | |
| Enthalpy of fusion (average)/kJ mol$^{-1}$ | 27.2 | | |
| $\Delta$Enthalpy$_{\text{(substituted-anthracene)}}$/kJ mol$^{-1}$ | −1.0 | | |
| Substituent (X = Br) | | | |
| Melting Point (average)/K: | | | 374.4 |
| $\Delta$MP$_{\text{(substituted-anthracene)}}$/K | | | −115.3 |
| Enthalpy of fusion (average)/kJ mol$^{-1}$ | | | 19.2 |
| $\Delta$Enthalpy$_{\text{(substituted-anthracene)}}$/kJ mol$^{-1}$ | | | −9.0 |
| Substituent (X = COOH) | | | |
| Melting point (average)/K: | 559.1 | | 495.6 |
| $\Delta$MP$_{\text{(substituted-anthracene)}}$/K | 69.4 | | 5.9 |
| Enthlapy of fusion (average)/kJ mol$^{-1}$ | 36.9 | | 34.7 |
| $\Delta$Enthalpy$_{\text{(substituted-anthracene)}}$/kJ mol$^{-1}$ | 8.7 | | 6.5 |
| Substituent (X = CHO) | | | |
| Melting point (average)/K: | | | 379.4 |
| $\Delta$MP$_{\text{(substituted-anthracene)}}$/K | | | −110.3 |
| Enthalpy of fusion (average)/kJ mol$^{-1}$ | | | 17.9 |
| $\Delta$Enthalpy$_{\text{(substituted-anthracene)}}$/kJ mol$^{-1}$ | | | −10.3 |

compound; Table 2 does so for single substituents and Table 3 compares those compounds with two heteroatoms. In each case, we show the ΔMP, or the change in melting point as the substituted anthracene minus pure anthracene's melting point. Interestingly, we see that the same heteroatom substituted can lead to a lower or higher melting point as compared to pure anthracene depending on the substituent's position. For example, 2-chloroanthracene has a melting point 6 K higher than anthracene, whereas the melting point of 1-chloroanthracene is over 100 K lower than anthracene [14]. Similarly, although the substituent group is the same for 2- and 9-anthracenecarboxylic acid, the melting point of 2-anthracenecarboyxlic acid is significantly higher, over 60 K higher, than its 9-carbon position counterpart. A possible reason for this is that the steric repulsion between the atoms in the molecule is smaller for the 2-anthracencarboxylic acid; the neighboring hydrogens are further away from the –COOH due to the outer angles of the outer aromatic ring for the 2nd position than the middle aromatic ring's angles of the 9th position. The carboxylic group, in both cases, leads to the formation of hydrogen bonds, which enhance molecular interactions (by strengthening the molecule); these stronger intermolecular interactions are seen through higher melting points than pure anthracene for both compounds. A similar trend noted by our laboratory for the enthalpy of sublimation is that the position of the heteroatom on the parent molecule plays an important role in shaping its thermodynamics. For example, the enthalpy of fusion for 2-anthracenecarboxylic acid is 36.9 kJ/mol, whereas for 9-anthracenecarboxylic acid it is 34.7 kJ/mol. Likewise, the enthalpy of sublimation for these compounds is 134.8 kJ/mol for 2-anthracenecarboxylic acid, 120.1 kJ/mol for 9-anthracenecarboxylic acid, and for pure anthracene is 98.5 kJ/mol [11, 15].

We see larger differences again at the 2-carbon position for 2-chloroanthracene versus 1-chloroanthracene. In this case, the melting point of the 2-chloroanthracene is slightly higher than that of anthracene (495.7 vs. 489.7 K, respectively) whereas the literature melting point of 1-chloroanthracene is 356.2 K [14]. Likewise, some of the largest effects noted for the substitution of two chlorines on anthracene are seen when one is in the 2-carbon position, though here we see extreme differences with compounds having both lower and higher melting points than the parent

**Table 3** Double heteroatom substitution effects of –Cl, –Br, and =O on anthracene

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Anthracene melting point/K | | | 489.7 | | | | |
| Anthracene enthalpy of fusion/kJ·mol$^{-1}$ | | | 28.2 | | | | |
|  | <br>Case 4 | <br>Case 5 | <br>Case 6 | <br>Case 7 | <br>Case 8 | <br>Case 9 | <br>Case 10 |
| Substituent (X = Cl) | | | | | | | |
| Melting point (average)/K: | 484.1 | 453.2 | 456.4 | 399.7 | 388.7 | 427.2 | 536.3 |
| $\Delta MP_{(\text{substituted-anthracene})}$/K | −5.6 | −36.5 | −33.3 | −90.0 | −101.0 | −62.5 | 46.6 |
| Enthalpy of Fusion (average)/kJ mol$^{-1}$ | 27.4 | | | | | | |
| $\Delta \text{Enthalpy}_{(\text{substituted-anthracene})}$/kJ mol$^{-1}$ | −0.8 | | | | | | |
| Substituent (X = Br) | | | | | | | |
| Melting Point (average)/K: | 495.4 | | 481.6 | | | | |
| $\Delta MP_{(\text{substituted-anthracene})}$/K | 5.7 | | −8.1 | | | | |
| Enthalpy of fusion (average)/kJ mol$^{-1}$ | 27.0 | | 32.1 | | | | |
| $\Delta \text{Enthalpy}_{(\text{substituted-anthracene})}$/kJ mol$^{-1}$ | −1.2 | | 3.9 | | | | |
| Substituent (X = O) | | | | | | | |
| Melting point (average)/K: | 557.3 | | | | | | |
| $\Delta MP_{(\text{substituted-anthracene})}$/K | 67.6 | | | | | | |
| Enthalpy of fusion (average)/kJ mol$^{-1}$ | 32.9 | | | | | | |
| $\Delta \text{Enthalpy}_{(\text{substituted-anthracene})}$/kJ mol$^{-1}$ | 4.7 | | | | | | |

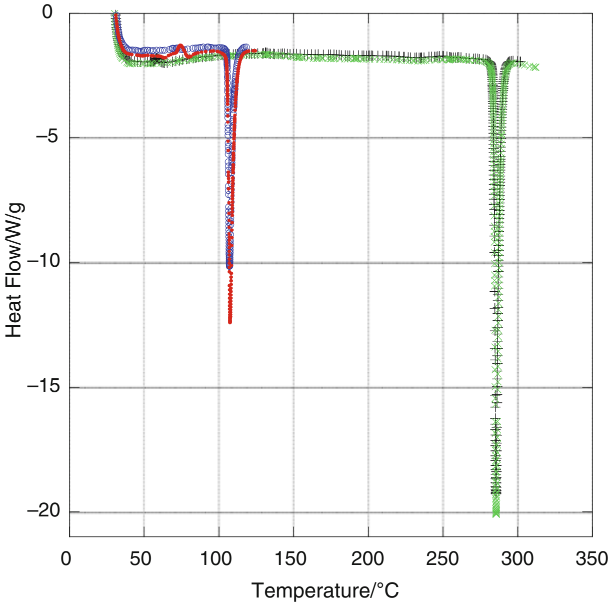


**Fig. 1** DSC profiles for two trials each of 9-anthraldehyde and anthraquinone (*red*) *closed circle* 9-anthraldehyde trial 1; (*blue*) *open circle* 9-anthraldehyde trial 2; (*black*) + anthraquinone trial 1; (*green* ) x anthraquinone trial 2

compound. For the 2,3-dichloroanthracene, the literature average melting point is 534.2 K [14, 16, 17], an increase over the parent compound of about 46 K. For 2,10-dichloroanthracene, we see a significant decrease in melting point, Tanimoto et al. [14] report a melting point between 388 and 389 K, over 100 K lower than that of anthracene, the largest decrease in melting point noted for any of the binary substituent compounds. Interestingly, the compounds with two chlorine heteroatom substitutions all have lower melting points (ranging from 5.6 to 101 degrees lower) than anthracene, except for the 2,3-dichloroanthracene. The smallest decrease is noted for the 9,10-dichloranthracene followed by the 1,5- and then 1,4-dichloroanthracene (with melting point depressions as compared to anthracene of −5.6, −33.3, and −36.5 K, respectively.)

Along the same line, the melting points of 1,5- and 9,10-dibromoanthracene are fairly close to unsubstituted anthracene, differing by −8.1 and +5.7 K, respectively. In the case of the 9,10-substitutions, the molecular polarity is smaller as compared to the 1,5-substitutions, such that the polarization is more localized. Here, we likely see slightly more molecular repulsion in the case of the 1,5-substitutions (resulting in slightly lower melting points than pure anthracene) as the hurdle to escape the condensed phase is lowered.

For the case of 9,10-carbon substitutions, the melting point increases as the molecular mass of the substituents group increases from –Cl to –Br to =O (as seen through 9,10-dichloroanthracene, 9,10-dibromoanthracene, and anthraquinone). When the substituent group is the ketone, as in anthraquinone, the 3-ring aromatic system likely breaks into two separate aromatic units leading to less $\pi$–$\pi$ interactions. However, the electronegativity also increases, which appears to dominate the molecular interactions in this case; the electronegativity of bromine is the lowest of these three substituents and the bromine appears to influence the melting point the least, followed by chlorine and then oxygen, while we see the largest difference in melting point for the anthraquinone. This is intuitive as the higher electronegativity of the oxygen molecules are more likely to attract bonding pairs, resulting in stronger interactions and therefore a higher melting point and enthalpy of fusion.

We see an expected trend for both the enthalpy of fusion and sublimation as compared to melting point. Figure 2 shows this relationship; as melting point increases, so does the heat required to change the phase of the component from solid to liquid and vapor. The relationship is slightly better for the enthalpy of sublimation ($\Delta H_{\mathrm{sub}}$) versus melting point in terms of statistical significant (an $R$ value of 0.899 as compared to 0.657 for melting point and fusion enthalpy, $\Delta H_{\mathrm{fusion}}$) as described by Fig. 2. These correlations suggest that the enthalpy of sublimation increases faster with melting point temperature than does the enthalpy of fusion. The two enthalpies of sublimation that sit considerably lower than the trendline in Fig. 2 are the data points for anthracene and 2-chloroanthracene whereas the outlier at the top right, with an enthalpy considerably higher than the trendline predicts, is 2-anthracenecarboxylic acid.

The 2-carbon position of anthracene creates issues when it comes to modeling the effects of heteroatoms. We observe this here with fusion studies and have seen it previously with sublimation studies [11, 18]. We surmise

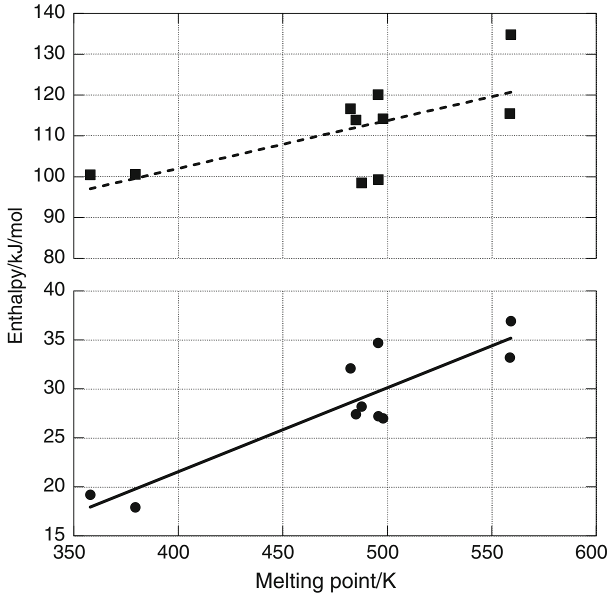


**Fig. 2** Enthalpies of fusion (*filled circle*) and sublimation (*filled square*) [11, 15, 18] versus melting point for heteroatom substituted anthracene compounds measured in this laboratory

that this is the effect of both inter- and intra-molecular interactions as not one explanation fits all cases. The potential exists for strong van der Waals, hydrogen bonding, and dipole–dipole interactions with the substituent at this position that could promote or hinder phase change depending on the heteroatom attached.

## Conclusions

The present study details the melting points and enthalpies of fusion of 10 polycyclic aromatic compounds with anthracene-based structures. The results for pure anthracene show excellent agreement with available literature data. We find no apparent trend between the fusion thermodynamics of these compounds and basic characteristics, such as molecular mass. Like other thermodynamic descriptions, the enthalpy of fusion of these substituted PAC is highly dependent on the type, number, and position of heteroatoms present in the molecule. A given heteroatom, depending on its substituent position, may increase or decrease the melting point as compared to the parent anthracene.

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