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Report

Melting Point, Boiling Point, and Symmetry

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The relationship between the melting point of a compound and its chemical structure remains poorly understood. The melting point of a compound can be related to certain of its other physical chemical properties. The boiling point of a compound can be determined from additive constitutive properties, but the melting point can be estimated only with the aid of nonadditive constitutive parameters. The melting point of some non-hydrogen-bonding, rigid compounds can be estimated by the equation

$$\mathrm{MP} = 0.772 * \mathrm{BP} + 110.8 * \mathrm{SIGMAL} + 11.56 * \mathrm{ORTHO} + 31.9 * \mathrm{EXPAN} - 240.7$$

where MP is the melting point of the compound in Kelvin, BP is the boiling point, SIGMAL is the logarithm of the symmetry number, EXPAN is the cube of the eccentricity of the compound, and ORTHO indicates the number of groups that are ortho to another group.

KEY WORDS: melting point; boiling point, symmetry; solubility.

INTRODUCTION

Despite the enormous amount of available melting point data, there are very few useful guidelines for understanding the relationship between the melting point of a compound and its chemical structure. In fact, it is sometimes difficult to tell if a compound is a solid or a liquid before it is isolated. The melting point of a compound is related to certain of its other physical chemical properties. Yalkowsky and Valvani have quantitatively related the solubility of a compound to its melting point and partition coefficient (1).

$$\log S_m = -\frac{\Delta S_f(\mathrm{mp} - 25)}{1364} - \log P + 0.8 \quad (1)$$

For the solubility of a compound in water to be estimated, it is necessary to know the melting point, entropy of fusion and the partition coefficient of the compound. Yalkowsky has shown that for many organic compounds, it is possible to estimate the entropy of fusion with reasonable accuracy (2). The log octanol–water partition coefficient can be estimated by group contribution methods (3,4). Since the entropy of fusion and the partition coefficients of organic solutes in water can be estimated, the solubility of organic compounds can be estimated with a knowledge of the melting point of the compound.

It is important to know the solubility of a compound in water before it is synthesized or available in sufficient purity for analytical measurements. It thus would be very useful to be able to estimate the melting point of a compound from its chemical structure. Techniques for the estimation of the melting point of organic compounds also would make available to the medicinal chemist methods for designing new drugs with a specified melting point range and therefore a specified solubility (5). Usually drugs with low melting points and high solubilities would be preferred, because of the increased dissolution rate. However, it is also possible to design drugs with higher melting points and therefore lower solubilities. A drug with a lower solubility may be useful for chewable tablets of a bitter substance. A drug with a lower solubility may have a lower dissolution rate and a prolonged activity. Compounds with low melting points can also cause problems with the pharmaceutical scientists involved with formulation, for example, liquids are difficult to formulate in solid dosage forms and may be difficult to isolate in an analytically pure form.

Although the boiling point of a compound can be determined from additive constitutive properties, its melting point cannot. There are many examples of isomers that have widely divergent melting points. The relationship between the structure of an organic compound and its boiling point has been investigated for over 100 years. Current techniques for the estimation of the boiling points of organic compounds are reviewed by Rechsteiner (6). In all the examples of boiling point estimation techniques, the boiling point is estimated from some form of an additive group contribution approach. The boiling point is used as the first estimator of melting point in order to see the influence of additive constitutive properties, which can be related to the enthalpy of melting. From this initial estimation using boiling point, geometric factors, which can influence the entropy of melting, are added.

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METHODS

Data Set. The compounds studied were all non-hydrogen-bonding substituted benzene molecules. These compounds were chosen because of their similar intermolecular interactions (no hydrogen-bonding groups), but the compounds cover a wide range of symmetry and melting point. Literature values for the melting points and boiling points of 85 non-hydrogen-bonding rigid compounds were obtained from the *CRC Handbook of Chemistry and Physics* (7). These compounds include fluoro, chloro, bromo, iodo, nitro, methyl, and nitrile substituted benzene derivatives.

Statistical Analysis. A data base for all the compounds used in this study has been developed on dBASE III software on Dec Rainbow and IBM compatible computers. Statistical analysis was performed using the multiple regression programs in SAS (8). The r values were used as a measure of correlation for each equation tested. Values above 0.9 were considered to be quantitatively useful, while values above 0.8 were considered to be useful for predicting trends but not for quantitative predictions. The t values were used in order to determine the significance of each independent variables contribution toward the whole multiple regression equation. t values greater than 4 were considered to be significant predictors, while values above 2 were considered to be of borderline significance.

Variables. One purpose of this study was to determine whether the melting point of a compound is dependent on additive constitutive properties of the molecule. Molecular properties rather than bulk properties were chosen along with the boiling point of a compound so that they can be used for predictions for compounds that have not yet been synthesized and for little studied compounds. Molecular properties are much more valuable in explaining discovered relationships. The boiling point of a compound can be estimated from additive molecular properties.

The rotational symmetry number of a molecule, σ, accounts for the statistical likelihood of finding a molecule properly oriented for incorporation into the crystal. The value of σ is calculated as the number of orientations of the molecule indistinguishable from a reference position. A methyl group is treated as symmetrical in this definition. In this report, polyatomic groups such as nitro and cyano are treated as monosubstituted groups that are coplanar with the benzene ring. In calculating the symmetry number of a molecule, the following groups are considered to be equal in size and shape: methyl, chloro, bromo, nitro, and cyano. The justification for using this system of equal size for the above groups is based on the positional disordering of crystals of rigid molecules. It is possible for a molecule without a center of symmetry to form centrosymmetric crystals. The space lattice of such crystals will have an equal number of points facing in opposite directions. Disordered rigid crystals such as these can be formed only when both crystal arrangements have similar energy. For example, *p*-chlorobromobenzene and *p*-nitrochlorobenzene have been found through X-ray diffraction analysis to form such crystals (9). The fluoro atom is considered to be equal in size to the hydrogen atom. Thus, for example, ortho-, meta-, and parabromochlorobenzenes have values of 2, 2, and 4, respectively, while ortho-, meta-, and parachloroiodobenzenes have values of 1, 1, and 2, respectively. The logarithm of σ is known as SIGMAL.

The variable ORTHO is an indicator variable which shows the number of functional groups that are ortho to another group. Ortho interactions are important in structure-property correlations in showing the significance of steric forces. As before, the fluorine atom is considered to be equal to the hydrogen atom and, therefore, is not counted in ortho interactions.

The eccentricity of a molecule is defined as the ratio of the maximum molecular length to the mean molecular diameter.

$$\text{Eccentricity} = \frac{\text{maximum molecular length}}{\text{mean molecular diameter}} \tag{2}$$

The mean molecular diameter is calculated as the diameter of a sphere occupied by the total volume of the molecule. Equation (3) gives the formula for the volume of a sphere.

$$\text{Volume} = \frac{4\pi r^3}{3} \tag{3}$$

Rearrangement of Eq. (3) and substituting Diameter/2 for the radius gives Eq. (4).

$$\text{Diameter} = 2\left[\frac{3(\text{volume})^{1/3}}{4\pi}\right] \tag{4}$$

The total volume of the molecule is calculated from the group contribution values from Edward (10). The maximum molecular length was determined from molecular models.

EXPAN, which is the eccentricity of the molecule to the third power, can be calculated now by substituting Eq. (4) into Eq. (1) and taking the entire quantity to the third power.

$$\text{EXPAN} = \frac{\pi(\text{length})^3}{6(\text{volume})} \tag{5}$$

RESULTS AND DISCUSSION

Melting Point. Since the change in free energy of a substance is equal to zero at its melting point, the melting point

Table I. Boiling and Melting Points of Isomers

Compound	MP	BP
1,2-Dichlorobenzene	−17	179
1,3-Dichlorobenzene	−25	172
1,4-Dichlorobenzene	53	175
1,2-Dibromobenzene	7	225
1,3-Dibromobenzene	−7	220
1,4-Dibromobenzene	87	220
1,2-Diiodobenzene	27	286
1,3-Diiodobenzene	40	285
1,4-Diiodobenzene	132	285
1,2,3-Trichlorobenzene	53	218
1,2,4-Trichlorobenzene	17	213
1,3,5-Trichlorobenzene	63	208
Methylpropylketone	−78	102
Diethylketone	−40	101.7

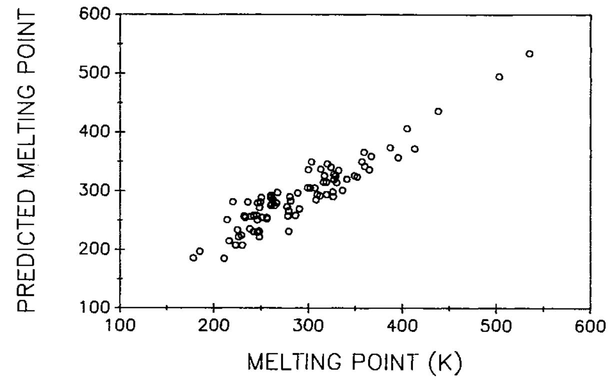

Fig. 1. Estimated melting points from Eq. (13).

in Kelvin can be related to the enthalpy of fusion, ΔH_f, and the entropy of fusion, ΔS_f, by the following relationship.

$$\mathrm{MP} = \frac{\Delta H_f}{\Delta S_f} \tag{6}$$

Therefore, the estimation of the melting point of an organic compound can be accomplished by the estimation of both the enthalpy of fusion and the entropy of fusion. The melting point will therefore be increased by any factor that raises the enthalpy of fusion or lowers the entropy of fusion. The effects of chemical constitution on the melting point of a compound can best be understood in terms of intermolecular forces and molecular geometric factors that can influence both the enthalpy of melting and the entropy of melting, respectively. The melting point of a compound is primarily governed by the intermolecular attractive forces that are present in a condensed collection of molecules. These forces can be thought of as the same forces that influence the boiling point of a compound. However, because of the close separation distances among molecules in a crystal, and the unknown crystal structure, these forces can not be interpreted as directly in the gas phase.

Entropy of Fusion. The entropy of fusion, ΔS_f, is related to the probability of melting by the Boltzmann relationship:

$$S_f = -R\ln(Pm) \tag{7}$$

The probability of melting can be thought of as the ratio of the number of arrangements, orientations, and conformations that are possible in the liquid to the much smaller number that are possible in the crystal. This is equivalent to the probability of a collection of molecules in the liquid phase meeting the geometric requirements of the crystal. An assumption is made that the molecules in a liquid have complete conformational and rotational freedom. The probability of melting then depends upon the rotational and conformational restrictions present within the crystal lattice.

The total entropy of fusion of rigid aromatic hydrocarbons is given by Eq. (8).

$$\Delta S_{\text{fusion}} = \Delta S_{\text{pos}} + \Delta S_{\text{exp}} + \Delta S_{\text{rot}} \tag{8}$$

The first term on the right-hand side of Eq. (8) is the positional entropy of fusion. The positional entropy of fusion is related to the change from the ordered arrangement of the molecular centers of gravity in the crystal to the random arrangement in the melt. Statistical mechanic treatment of the positional entropy of fusion has led to a calculated value of 2 to 3 eu (entropy units) (11,12).

The second term on the right-hand side of Eq. (8) is the entropy of expansion. The entropy of expansion is found to be between 1 and 3 eu for most rigid aromatic organic compounds (13). Compounds with a high eccentricity will have a large increase in volume upon melting and therefore have a large entropy of expansion. The entropy of expansion can be calculated from the following equation:

$$\Delta S_{\text{exp}} = R\ln\left[V(f)_{\text{liq}}/V(f)_{\text{solid}}\right] \tag{9}$$

where $V(f)$ corresponds to the free volume in either the liquid or the solid. Bondi (13) has called this the fluctuation volume. The last term in Eq. (8) is the entropy of rotation. The entropy of rotation is the change from the ordered arrangement of molecular centers in the crystal to the randomly oriented arrangement in the liquid. The rotational entropy of fusion for most rigid compounds is found to be 7 to 11 eu.

The geometric factor that can be most directly related to the probability of rigid molecules melting is the rotational

Table II. Summary of Regression Analyses

Parameter	Estimate	*T*	SIG	*N*	SD	*R*
		(A) Equation (11)				
BP	0.848	10.71	0.0001	85	41.6	0.763
Intercept	−105.7	−2.8	0.0058			
		(B) Equation (12)				
BP	0.952	18.2	0.0001	85	27.1	0.908
SIGMAL	113.0	10.7	0.0001			
Intercept	−206.2	−7.9	0.0001			
		(C) Equation (13)				
BP	0.772	13.9	0.0001	85	22.8	0.938
SIGMAL	110.8	12.4	0.0001			
EXPAN	31.9	5.5	0.0001			
ORTHO	11.5	5.3	0.0001			
Intercept	−234.4	−8.9	0.0001			

Table III. Boiling Point, Melting Point, Predicted Melting Point from Eq. (13), Residual, SIGMAL, EXPAN, and ORTHO for Each Compound in the Analyses

Compound	BP	MP	PRED	RES	SIGMAL	EXPAN	ORTHO
Benzene	353	279	231	47	1.08	2.3	0
Toluene	383	178	185	−7	0.30	2.8	0
1,3-Dimethylbenzene	412	226	221	5	0.30	3.3	0
1,2-Dimethylbenzene	417	248	221	27	0.30	2.4	2
1,4-Dimethylbenzene	411	286	258	28	0.60	3.4	0
1,3,5-Trimethylbenzene	438	220	281	−60	0.78	2.8	0
1,2,4-Trimethylbenzene	442	229	224	5	0.00	3.0	2
1,2,3-Trimethylbenzene	449	248	271	−23	0.30	2.8	3
1,2,3,5-Tetramethylbenzene	471	249	280	−31	0.30	2.6	3
1,2,3,4-Tetramethylbenzene	478	267	297	−30	0.30	2.6	4
1,2,4,5-Tetramethylbenzene	470	352	324	28	0.60	2.6	4
Pentamethylbenzene	503	327	319	8	0.30	2.3	5
Hexamethylbenzene	537	438	436	2	1.08	2.1	6
Nitrobenzene	483	279	266	13	0.30	3.0	0
2-Nitromethylbenzene	495	262	285	−23	0.30	2.5	2
3-Nitromethylbenzene	505	288	296	−8	0.30	3.4	0
4-Nitromethylbenzene	511	324	340	−16	0.60	3.6	0
Iodobenzene	461	242	258	−16	0.30	3.2	0
3-Iodomethylbenzene	486	246	250	−4	0.00	3.4	0
4-Iodomethylbenzene	484	309	294	15	0.30	3.8	0
1,2-Diiodobenzene	559	300	336	−36	0.30	2.6	2
1,3-Diiodobenzene	558	313	337	−24	0.30	3.4	0
1,4-Diiodobenzene	558	405	406	−1	0.60	4.5	0
Bromobenzene	429	242	230	12	0.30	3.1	0
3-Methylbromobenzene	457	233	254	−20	0.30	3.2	0
2-Methylbromobenzene	455	245	258	−13	0.30	2.7	2
4-Methylbromobenzene	458	302	305	−4	0.60	3.7	0
3-Bromoiodobenzene	525	264	275	−11	0.00	3.3	0
4-Bromoiodobenzene	524	365	336	29	0.30	4.2	0
3-Dibromobenzene	493	266	279	−13	0.30	3.1	0
2-Dibromobenzene	498	280	290	−10	0.30	2.6	2
4-Dibromobenzene	493	360	342	18	0.60	4.1	0
1,3,5-Tribromobenzene	544	395	357	38	0.78	2.7	0
1,2-Dimethyl-tetrabromobenzene	647	535	534	1	1.08	2.5	6
Chlorobenzene	405	223	207	16	0.30	3.0	0
3-Methylchlorobenzene	435	225	233	−7	0.30	3.1	0
2-Methylchlorobenzene	431	238	235	3	0.30	2.5	2
4-Methylchlorobenzene	435	281	283	−3	0.60	3.6	0
2-Chloronitrobenzene	518	307	305	3	0.30	2.6	2
3-Chloronitrobenzene	509	319	294	25	0.30	3.2	0
4-Chloronitrobenzene	515	357	350	7	0.60	3.8	0
4-Chloroiodobenzene	500	330	314	16	0.30	4.0	0
3-Chlorobromobenzene	469	251	254	−3	0.30	2.9	0
2-Chlorobromobenzene	477	261	277	−16	0.30	2.7	2
4-Chlorobromobenzene	469	341	320	22	0.60	3.9	0
1,3-Dichlorobenzene	445	248	231	18	0.30	2.8	0
1,2-Dichlorobenzene	452	256	254	3	0.30	2.6	2
1,4-Dichlorobenzene	448	326	298	29	0.60	3.7	0
3,5-Dichloromethylbenzene	474	299	305	−5	0.78	2.7	0
3,4-Dichloro-1,2-dimethylbenzene	507	349	326	23	0.30	2.8	4
2,4-Dichloromesitylene	516	332	335	−3	0.30	2.5	5
1,2,4-Trichlorobenzene	486	290	269	21	0.00	3.3	2
1,2,3-Trichlorobenzene	491	326	290	36	0.30	2.4	3
1,3,5-Trichlorobenzene	481	336	301	35	0.78	2.4	0
2,3,4-Trichlorotoluene	505	317	326	−9	0.30	2.9	4
2,3,5-Trichlorotoluene	504	319	315	4	0.30	2.9	3
1,2,3,4-Tetrachlorobenzene	527	320	346	−26	0.30	3.0	4
1,2,4,5-Tetrachlorobenzene	517	413	372	41	0.60	3.0	4
Pentachlorobenzene	549	359	366	−6	0.30	2.7	5
Hexachlorobenzene	599	503	495	9	1.08	2.4	6
Fluorobenzene	358	232	257	−25	1.08	3.0	0

Table III. Continued

Compound	BP	MP	PRED	RES	SIGMAL	EXPAN	ORTHO
1,3-Fluoromethylbenzene	389	185	196	−11	0.30	3.0	0
1,2-Fluoromethylbenzene	387	211	184	27	0.30	2.7	0
4-Fluoromethylbenzene	390	216	214	2	0.30	3.6	0
4-Fluoroiodobenzene	456	246	279	−33	0.30	4.0	0
4-Fluorobromobenzene	425	256	252	5	0.30	3.9	0
2-Chlorofluorobenzene	411	230	207	23	0.30	2.8	0
4-Chlorofluorobenzene	403	246	229	17	0.30	3.7	0
1,3-Difluorobenzene	356	214	250	−36	1.08	2.8	0
1,2-Difluorobenzene	364	239	256	−17	1.08	2.8	0
1,4-Difluorobenzene	368	260	288	−28	1.08	3.7	0
1,2,3,5-Tetrachlorobenzene	519	327	328	−1	0.30	3.0	3
Hexafluorobenzene	354	278	257	22	1.08	3.1	0
1,2,4,5-Tetrafluorobenzene	362	277	273	5	1.08	3.4	0
1-Fluoro-2,4,6-trimethylbenzene	442	236	281	−44	0.78	2.7	0
Benzonitrile	464	260	275	−15	0.30	3.7	0
2-Bromobenzonitrile	524	329	325	3	0.30	3.1	2
3-Bromobenzonitrile	498	312	292	20	0.30	3.4	0
4-Bromobenzonitrile	508	387	374	13	0.60	4.7	0
2-Chlorobenzonitrile	505	316	315	1	0.30	3.2	2
4-Chlorobenzonitrile	496	367	359	8	0.60	4.5	0
4-Fluorobenzonitrile	462	308	285	23	0.30	4.1	0
2-Methylbenzonitrile	478	260	292	−33	0.30	3.2	2
3-Methylbenzonitrile	486	250	288	−38	0.30	3.6	0
4-Methylbenzonitrile	491	303	349	−47	0.60	4.3	0

symmetry. The more symmetrical isomers melt higher than the less symmetrical ones. This is from a combination of a lower rotational entropy of fusion and a higher packing efficiency, both of which raise the melting point.

SIGMAL is the logarithm of the rotational symmetry number of the molecule. In calculating the symmetry number of a molecule, the following groups are considered to be equal in size:

$$\text{methyl} = \text{chloro} = \text{bromo} = \text{cyano} = \text{nitro} \qquad (10)$$

From an intuitive point of view, molecular symmetry is a measure of the probability that a freely rotating molecule will be oriented in a manner suitable for incorporation into the crystal. This definition of SIGMAL will help explain the orientational disordering of crystals. From Eq. (7), it is apparent that the logarithm of the symmetry number will give a better correlation with melting point than the symmetry number.

Table I gives the melting point and boiling point of some organic compounds. It can be seen from this table that symmetrical compounds melt at a much higher temperature than their less symmetrical isomers. On the other hand, isomers generally have similar boiling points with the symmetrical compound boiling at a slightly reduced temperature. The reason for this lowering of the boiling point with symmetry is that for compounds with a functional group, the Debye and Keesom forces will increase according to the net dipole moment. Symmetrical molecules generally have lower net dipole moments. In a condensed phase such as a liquid the Debye and Keesom forces act over very short distances. Therefore, it is the scalar dipole moment that is important. Each group in the molecule will act as an independent dipole. The net dipole moment of the molecule will only have a very small effect on the total energy. The net dipole moment will favor very slightly the ortho substituted benzene derivatives that are found to have a higher boiling point than the para substituted compounds, which have either no dipole moment or a small dipole moment. From Table I it is clear that the ortho substituted benzene derivatives have a higher boiling point than the meta or para. The 1,2,3-trisubstituted compound, with its increased dipole moment, also shows a higher boiling point than the other two trisubstituted compounds. The more symmetrical isomers such as the symmetrical ketone also have a lower boiling point.

The melting points of 85 non-hydrogen-bonding compounds were correlated with their boiling points and symmetry numbers in order to study the effect of symmetry on the melting point of organic compounds. Only rigid, non-hydrogen-bonding compounds were selected in this data set.

The following equation correlates the melting point (K) and the boiling point (K) of benzene derivatives:

$$\text{MP} = 0.848 * \text{BP} - 105.7 \qquad (11)$$
$$r = 0.763, \quad n = 85, \quad s = 41.6$$

where MP is the melting point of the compound in Kelvin and BP is the boiling point of the compound in Kelvin. From the standard deviation, it is clear that there is a great variance in the data.

The next step of the analysis was to correlate the melting point with the boiling point and the logarithm of the symmetry number of the molecule (SIGMAL).

$$\text{MP} = 0.952 * \text{BP} + 113.0 * \text{SIGMAL} - 206.2 \qquad (12)$$
$$r = 0.908, \quad n = 85, \quad s = 27.1$$

The final step in this analysis was to correlate the melting point with the boiling point, SIGMAL, EXPAN, and ORTHO:

$$\begin{aligned} \mathrm{MP} = {} & 0.772 * \mathrm{BP} + 110.8 * \mathrm{SIGMAL} + 11.56 * \mathrm{ORTHO} \\ & + 31.9 * \mathrm{EXPAN} - 234.4 \\ & r = 0.938, \quad n = 85, \quad s = 22.8 \end{aligned} \tag{13}$$

Figure 1 shows the predicted melting point from Eq. (13) against the actual melting point. From Fig. 1 it is clear that Eq. (13) gives an excellent correlation with melting point. A summary of the regression analyses is contained in Table II. Table III lists the boiling point (BP), melting point (MP), predicted melting point (PRED) from Eq. (13), and residual (RES) for each compound in the analyses. The melting points and boiling points in this table are actual values from the *CRC Handbook of Chemistry and Physics*. Table III also contains the data for EXPAN, ORTHO, and SIGMAL.

In order to determine the appropriateness of introducing a four-parameter equation [Eq (13)] over the simpler two-parameter Eq. (12), both an F test and Akaike's information criterion test (AIC) were performed on the data. Both tests showed that Eq. (13) was superior to Eq. (12). A correlation of melting points using just the geometric factors and excluding the boiling point was also attempted.

$$\begin{aligned} \mathrm{MP} = {} & 86.5 * \mathrm{SIGMAL} + 29.8 * \mathrm{ORTHO} \\ & + 63.0 * \mathrm{EXPAN} + 20.5 \\ & r = 0.767, \quad n = 85, \quad s = 41.8 \end{aligned} \tag{14}$$

CONCLUSION

In conclusion, simple equations have been developed that can estimate the melting point of a wide variety of non-hydrogen-bonding compounds from their boiling point and factors related to their geometry. The use of boiling point can be related to intermolecular forces that influence the enthalpy of melting. The geometric forces can be related to the entropy of melting. Neither the geometric factors nor the boiling point alone can estimate the melting point as seen in Eqs. (11) and (14).

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