

# Research on the Correlation Between the Lattice Enthalpy of Ionic Compounds and Melting Points

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**Abstract:** Ionic compounds own different crystal structures from molecular compounds due to the electrostatic force, generating affinities between cations and anions. The lattice energies are made strong and require large energy to break the solids. This paper is used to illustrate the influence of different factors on lattice enthalpy, and correlations between lattice enthalpy and melting points, Regarding carbon fibers as templates, trying to find out if there were theoretically possibilities to utilize ionic crystals more in industrial engineering. Several graphs are made based on the database. Research shows that ion charges are direct proportional to the strength of lattice energy; while ionic radius own inverse relationships. However, unexpected results have been found toward melting points, claiming no obvious effect is made by lattice energies. The reason might contribute to the ideal assumption in terms of lattice enthalpy, assuming they were all in perfect form.

**Keywords:** Ionic crystals; Lattice enthalpy, Melting points, Ionic radius, Ion charges, Coulomb's Law, Carbon Fiber.

## 1. Introduction

The curiosity of this investigation came from when I reviewed a chemistry report on sports. Through reviewing the ideas illustrated in this article, different kinds of chemicals have been used in wear fabric, which is categorized as Textile Chemistry. However, It seems peculiar that there are rarely ionic compounds applied. In specific, those materials, for example, bioceramic fabric, hydro spider silk, and carbon fiber have been proven to perform well in the wear fabrics. Yet how about those ionic compounds? We all can see that compared with molecular compounds, the force applied in the lattice is much stronger, due to the ionic bonding, formed by the mutual affinity between anions and cations. The melting points, therefore, would be higher as well. Then several questions came: What has affected the strength of ionic lattice? Is it possible for us to utilize them as innovations to fabric chemistry? What can we do with this special and high boiling point? Are there any hidden benefits waiting for exploring? To be more specific, what factors may affect the strength of lattice enthalpy and how does it work? Do we have any chances to apply ionic lattice traits in the fabric chemistry field in sports? Also, the melting point is used to determine the purity of the ionic compound. The higher the purity, the functionality is stronger. so, I also want to investigate the correlation between the lattice enthalpy of ionic compounds and melting point.

## 2. Related Theories

### 2.1. The structure of the ionic compound

In general, ionic compounds are existed in a form of special solid, which specifically named lattices. The electrostatic force of attraction between positive and negative ions causes the ions surround themselves with ions of opposite charge. So, the ionic compound takes on a predictable three-dimensional

crystalline structure, which is known as the ionic lattice. The lattice's geometry depends mainly on the radius of the ions, so the geometries vary in different compound. But different compounds have a fixed arrangement of ions based on a repeating unit. For instance, the coordination number of NaCl is 6, each Na<sup>+</sup> ion is surrounded by six Cl<sup>-</sup> ions and each Cl<sup>-</sup> ion is surrounded by 6 Na<sup>+</sup> ions.[1]

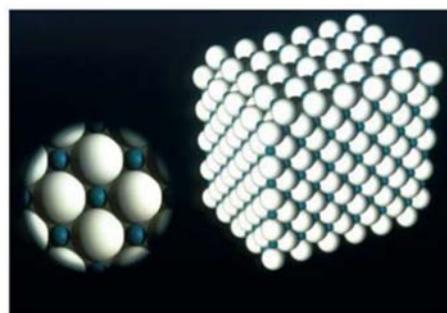
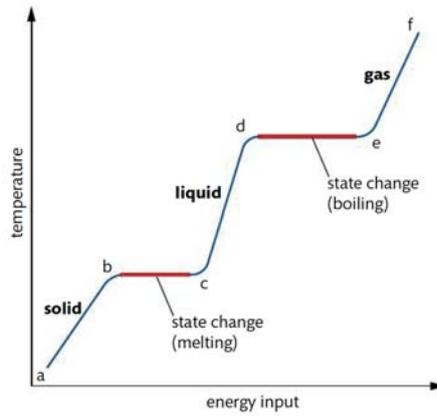


Figure 1. The lattice structure of the ionic compound [1]

### 2.2. The melting point of the ionic compound

Melting point is the temperature at which a given solid material changes from a solid state to a liquid, or melts. When the heat is applied to a solid, the vibrational energy of its particles increases and the temperature increases. When the temperature reaches the melting point, the solid start to melt. Also, more heat is needed to break the intermolecular force and convert all the solids into liquids without temperature change. When all the solids turn into the liquids, additional heat will be added to raise the kinetic energy and temperature of the liquid. The melting temperature of crystalline solids is a characteristic figure and is used to identify pure compounds and elements. [2] Most mixtures and amorphous solids melt over a range of temperatures. But the pure substance melts at a specific temperature.[3]

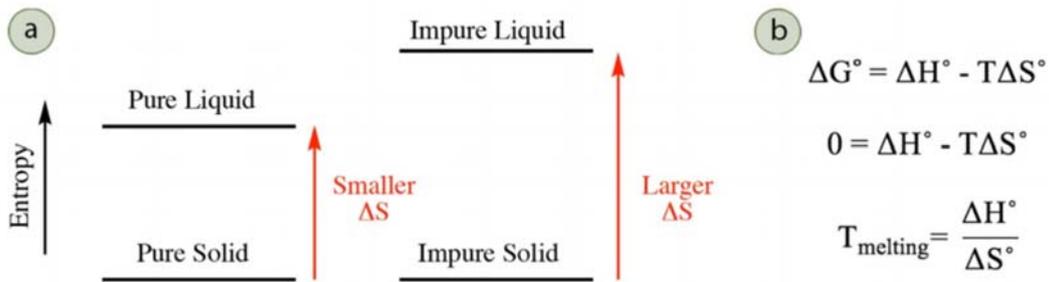


**Figure 2.** The heating curve of the solid to liquid and gas [1]

Many simultaneous attractions between cations and anions that occur, so the ionic crystal lattices are very strong. The process of melting the ionic compounds require large amounts of energy in order to break all of the ionic bonds in the crystal structure. Higher melting points compounds would help in lots of fields in industrial engineering.[4]

of the solid becomes a mixture of solid and liquid. Also, the solid and liquid phases are in equilibrium state (solid  $\rightleftharpoons$  liquid). As we know, when the system is at equilibrium, the change of Gibbs free energy is zero. The equation of  $\Delta G_o = \Delta H_o - T\Delta S_o$  (see figure 3), so the melting point :  $T = \frac{\Delta H}{\Delta S}$ . [5]

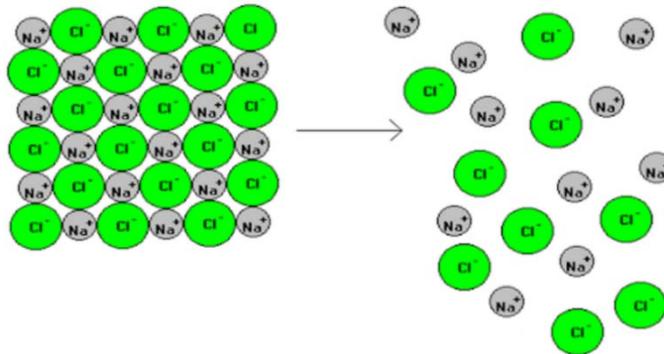
When the temperature reaches the melting point, the phase



**Figure 3:** The entropy changes during melting process and determination of melting point.[6]

Where  $\Delta H$  is the energy needed to melt one mole of ionic crystal;  $T$  is the melting point;  $\Delta S$  is the entropy change of the

system.



**Figure 4.** The ionic bonds are broken in NaCl ionic crystal melting process

$\Delta H$  (lattice enthalpy) is associated with atom radius and ionic charges and can represent the attraction force in the lattice structure. It may show a positive correlation with the melting point of the materials.[7]

Solids are restricted in atomic motion, there is little

difference in entropy between a pure and impure solid. An impure liquid has greater disorder and greater entropy, so there is a significant difference in entropy between a pure and impure liquid. So, the melting point of an impure solid is much larger than a pure solid.

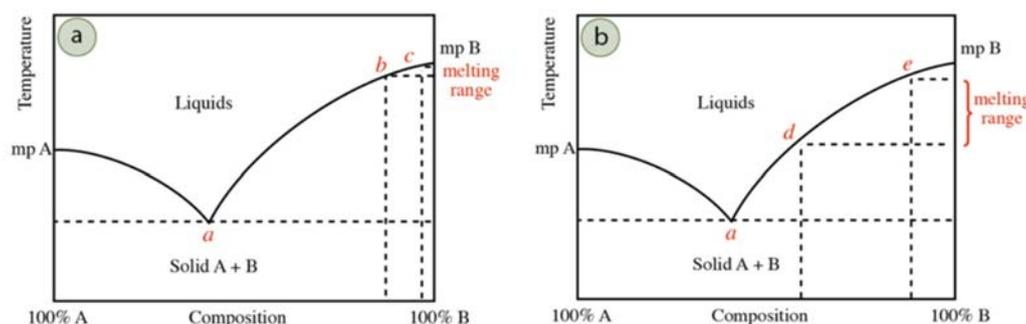
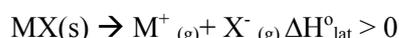


Figure 5. The melting process of pure and impure substance .[6]

### 2.3. The lattice enthalpy of the ionic compound

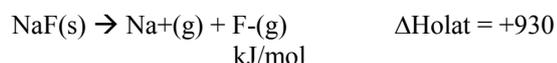
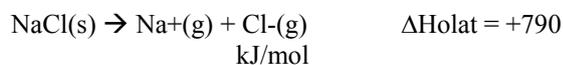
In the terms of lattice enthalpy, it is defined as the standard enthalpy change that occurs on the formation of 1 mol of gaseous ions from the solid lattice [1] :



The application of Coulomb's Law in the field of lattice enthalpy: both charges of cations and anions, and nucleus radius are considered to be factors that affect the strength of lattice enthalpy. Focusing on the forming of ionic compounds, they are made of positive and negative ions, particularly cations and anions. Those two ions are held together by electrostatic forces[8].

In addition, this compound is made neutral, the total charges of cations and anions would be kept the same to ensure the compound is stable. Since that, when the ionic radius of the ions in the compound, we can imagine with a higher charge from positive and negative sides, the attraction between ions would be stronger, resulting in a stronger ionic bond, larger lattice enthalpy. Same conclusion would be found when the ionic charges are similar, the distance between the positive ion and negative ion is smaller, then stronger force of electrostatic attraction will be, larger lattice enthalpy.

For instance:



The lattice enthalpies of ions can be determined by the ionic model under the assumption that the crystals are in perfectly spherical form. This ionic model assumes that the only interaction in the ionic compound is due to electrostatic forces between the opposite ions. The overall attraction between the positive and negative ions predominates over the repulsion of ions with the same charge as ions are generally surrounded by neighboring ions of opposite charge.

The only interaction between ions is the electrostatic force hence the energy needed to break such force is depending on the product of the ionic charges and the sum of the ionic radii. The general expression of lattice enthalpy is defined[1]:

$$\Delta H_{\text{lattice}}^{\ominus} = \frac{Knm}{R_{M^{n+}} + R_{X^{m-}}}$$

Where K is a constant depends on lattice geometry, n and m are the magnitude of charges on the ions.  $R_M$  and  $R_X$  are the ionic radii that can be measured by X-ray diffraction.

### 3. Methodology

Two independent variables were determined:

1. The ionic radius of cation and anion
2. The charge of cation and anion.

Dependent variable: The lattice enthalpy of group1 and group2 ionic compounds

Controlled variables: To investigate the effect of ionic radius on the lattice enthalpy, same group of metal salts are chosen. To investigate the correlation between the lattice enthalpy of ionic compounds and melting point, the same group metal with different halogens is chosen.

All the databases cited in this investigation are from reliable databases.

Table 1. Data Base Citation

Atomic radius	<p>“ChemSpider   Search and Share Chemistry.” Chemspider.com, 2019, www.chemspider.com. Accessed 4 Nov. 2019. [9]</p> <p>CHEMISTRY ATAR Course data booklet, Government of Western Australia, School Curriculum and Standards Authority, 2019.[10]</p> <p>Bryan, R. F. “Modern Crystallography, Vol. 2. Structure of Crystals Edited by B. K. Vainshtein, v. M. Fridkin and v. L. Indenbom.” Journal of Applied Crystallography, vol. 28, no. 6, 1 Dec. 1995, pp. 860–860, 10.1107/s0021889895099493. [11]</p>
Theoretical lattice enthalpy	<p>Chemical Index Database, Drug Information Express, Drug R&amp;D, Chemical Database [12]</p> <p>Diploma Programme Chemistry data booklet, International Baccalaureate Organization 2007.[13]</p>
Melting point	<p>Chemistry Data Booklet, Authority S Q. Access 3 Chemistry[J]. 2013.[14]</p> <p>Chemistry Data Booklet, national 5, Scottish Qualifications Authority. 2013.[15]</p>

This table is used to prove the data in these sources are reliable, because they're cited for many times.

## 4. Results and Analysis

### 4.1. Raw data

**Table 2.** Ionic radius of group1, group2 cations and group17 anions

Ionic radius 10-12m	Group1		Group1		Group17	
	Li+	76	Be2+	56	F-	133
	Na+	102	Mg2+	72	Cl-	181
	K+	138	Ca2+	100	Br-	196
	Rb+	152	Sr2+	118	I-	220
	Cs+	167	Ba2+	135		

**Table 3** The lattice enthalpy of different halide salts (Group 1)

Group1 metal halides	$\Delta H_{\text{lattice}}$ (kJ/mol)			
	F	Cl	Br	I
Li	1049	864	820	764
Na	930	790	754	705
K	829	720	691	650
Rb	795	695	668	632
Cs	759	670	647	613

**Table 4** The lattice enthalpy of different halide salts (Group 2)

Group2 metal halides	$\Delta H_{\text{lattice}}$ (kJ/mol)			
	F	Cl	Br	I
Be	3456	3033	2950	2780
Mg	2957	2540	2406	2293
Ca	2602	2271	2132	2074
Sr	2427	2170	2046	1984
Ba	2314	2069	1950	1890

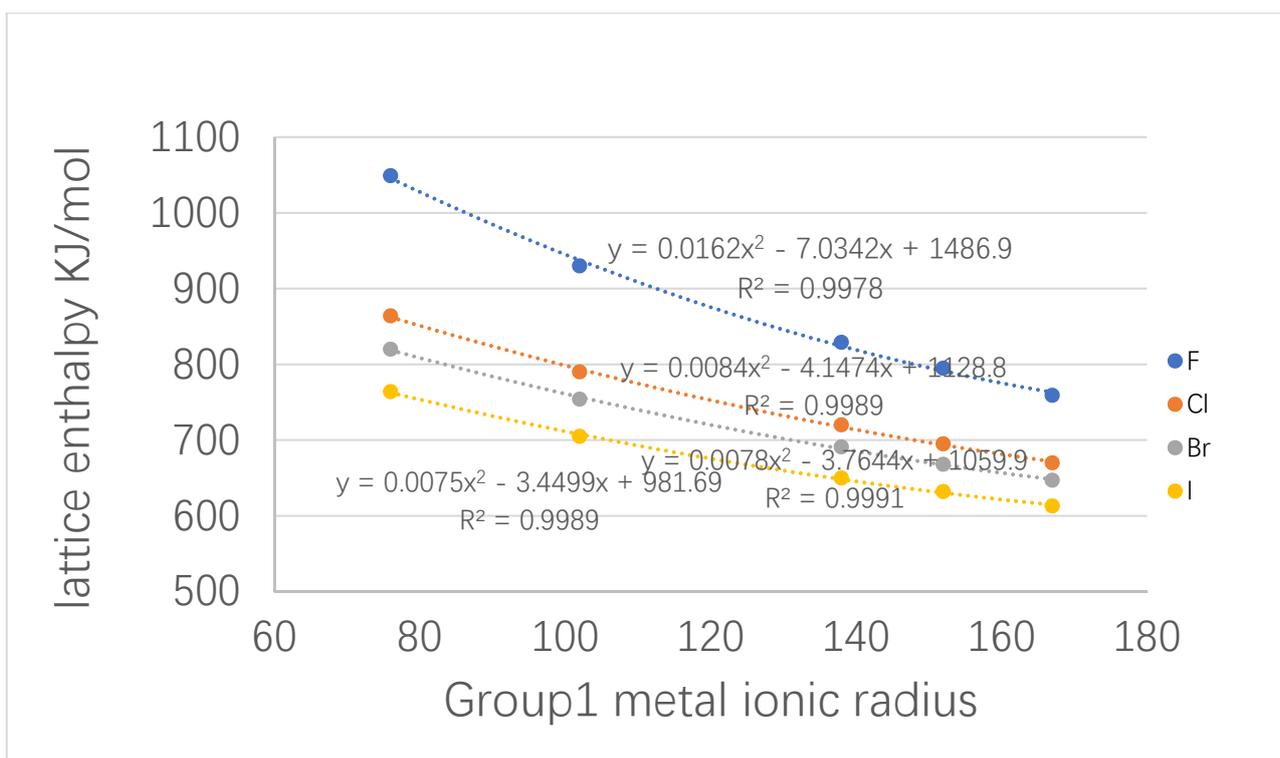
**Table 5** The melting point of different metal halide salts

Melting point of different metal halides °C				
	F	Cl	Br	I
Alkali metal halide				
Li	848	610	552	469
Na	993	801	747	661
K	858	770	734	681
Rb	795	718	693	647
Cs	682	645	636	621
Group2 metal halides				
Be	554	401	508	480
Mg	1263	714	711	637
Ca	1418	775	636	779
Sr	1477	874	643	540
Ba	1368	962	857	711

### 4.2. Graphing and graph interpretation

- 9 have been made.

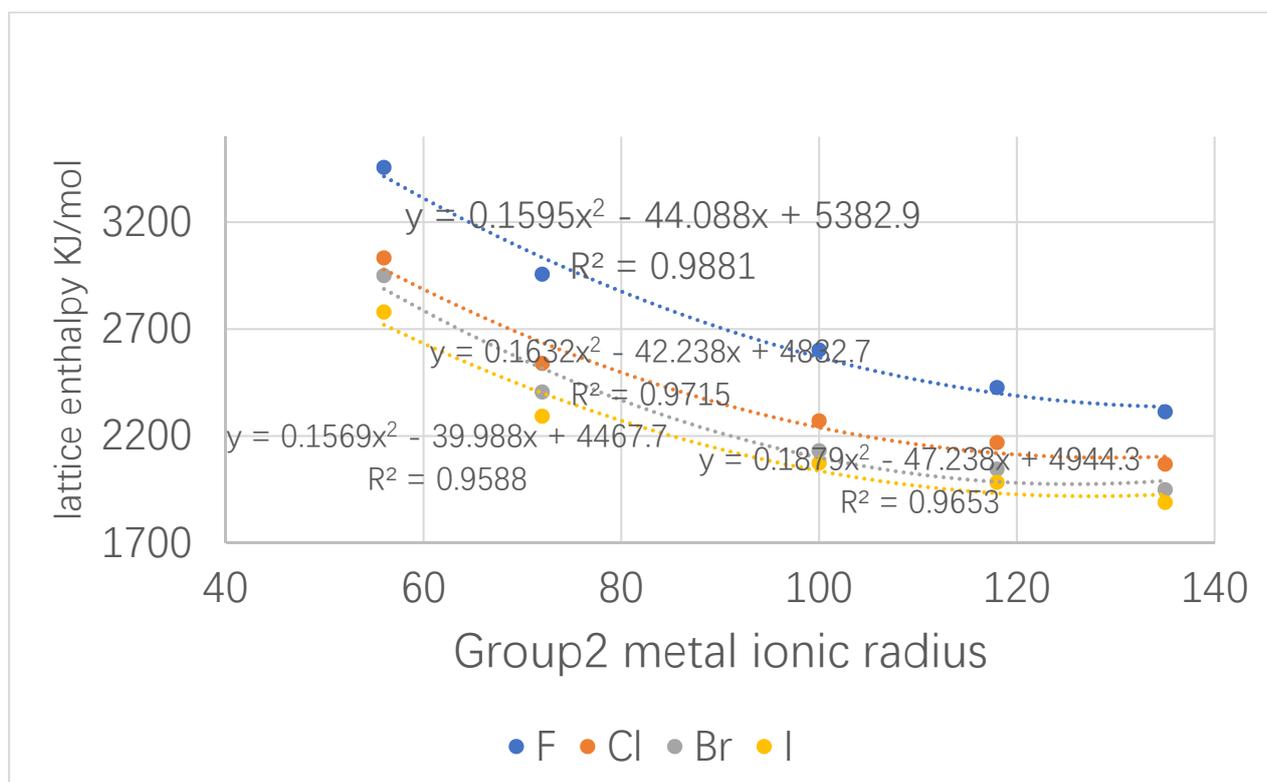
Based on the information shown from Table 2 - 5, Figure 6



**Figure 6.** The lattice enthalpy of group 1 metal salts with different halogens

From Figure 6, we can see similar trends that have been showed with ionic compounds that made of group 1 metal with different Halogens. It is obvious that as the metal ionic radius decreases, the lattice enthalpy of the compounds would increase, ranging from 1050 to nearly 750 KJ/mol. By focusing on the  $R^2$ , all those four are very close to 1, which

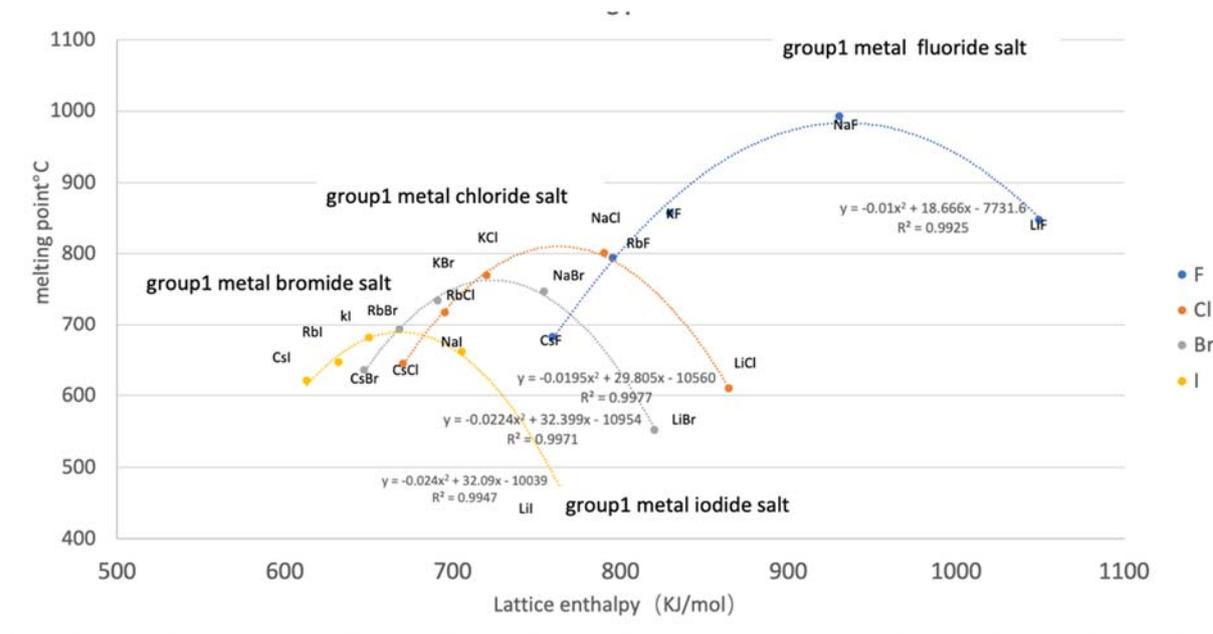
indicates an effective approach to the best fit line. According to the theories, as metal ionic radius increases, it means to an increasing distance between ions, so that the force of electrostatic attraction applied there would be weakened, followed by drops in the strength of ionic bond and the lattice enthalpy.



**Figure 7.** The lattice enthalpy of group 2 metal salts with different halogens

Figure 7 (Group 2 metal salt) shows a dropping tendency as Figure 6 (Group 1 metal salt). For example, when the same metal cation ( $\text{Be}^{2+}$ ) form salts with different halide, as the ionic radius increase from  $\text{F}^-$  ( $133 \times 10^{-12}\text{m}$ ) to  $\text{I}^-$  ( $220 \times 10^{-12}\text{m}$ ), the lattice enthalpy decrease form 3456 kJ/mol to 2780 kJ/mol. Similar trend is found that when same halide anion ( $\text{F}^-$ ) form salts with different metal cations, as the ionic radius

increase from  $\text{Be}^{2+}$  ( $56 \times 10^{-12}\text{m}$ ) to  $\text{Ba}^{2+}$  ( $135 \times 10^{-12}\text{m}$ ), the lattice enthalpy decrease form 3456 kJ/mol to 2314 kJ/mol. Apart from this, the range of the lattice enthalpy of compounds that made of group 2 metal salt is relatively higher than that of group 1 metal. This is not surprising in the case that group 2 metal salts own traits of smaller radius, means narrower gaps while forming compounds.

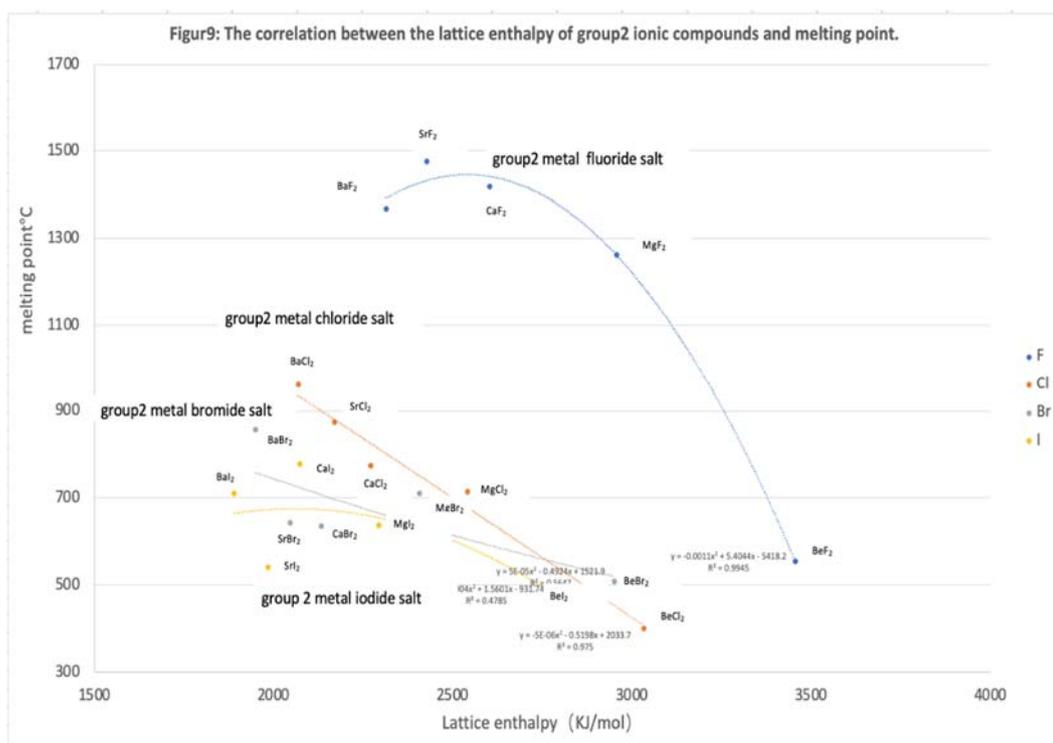


**Figure 8.** The correlation between the lattice enthalpy of group 1 ionic compounds and melting point

Figure 8 has showed a correlation between the lattice enthalpy and melting points of Group 1 ionic compounds. The correlation coefficient of fluoride, chloride, bromide and iodide is 0.58, -0.18, -0.43, -0.71, which shows there is a positive or negative correlation between the melting point and lattice enthalpy. For most of the salts, when the lattice enthalpy is larger, the melting point is larger. However, for NaF, NaCl, NaBr, NaI, KI don't follow the trend. There's a big increase of melting point while the lattice enthalpy is smaller. The possible reason maybe the covalent character of ionic bond. If covalent character of ionic compound increases melting point decreases. The covalent character of ionic bond arises due to the polarizing power of cation, but fluorine is more electronegative, so Na can't polarize fluorine and the other elements of the group form ionic compounds and due to less polarizing effect on fluorine we can consider lattice energy. The difference in the size of the ions will determine the percentage of covalent character in the ionic bond. For example, if the size of the cation is very small and that of the anion is very large. The ionic bond will show more covalent characters. However, lithium can polarize fluorine. so the covalent character of LiF forms, so its melting point will be

low.[16]

Figure 9 has showed a trend (the correlation between the lattice enthalpy and melting points of Group 2 ionic compounds) that are not well defined. The trend-lines are irregular compared with the graph showed in Figure 8, except for those combining with Fluorine. The  $R^2$  values are both close to 1 for ionic compounds with Fluorine and Chloride, yet only around 0.5 for that with Bromine and Iodine. This contradicts to the pattern we found in the past. Through investigating the paper edited by Christopher and Lydia,[17] the reason might because of the process of absorbing heat and destroying the bonds. In common, a higher lattice enthalpy typically means to have higher melting points. However, Beryllium halide has a lower melting point while the lattice enthalpy is largest. Also,  $\text{BaCl}_2$ ,  $\text{BaBr}_2$ ,  $\text{BaI}_2$  have higher melting point than  $\text{SrCl}_2$ ,  $\text{SrBr}_2$ ,  $\text{SrI}_2$  while the lattice enthalpy was lower. The possible reason maybe the the melting point of ionic solid is depends on lot of factors including ion packing, coordination geometry, and ionic character of the bond.[18]



**Figure 9.** Correlation between the lattice enthalpy of group2 ionic compounds and melting point

## 5. Conclusion

### 5.1. The aim of the experiment is to:

investigate the relationship between ionic radius, ionic charge and the lattice enthalpy

Investigate the correlation between lattice enthalpy and melting point.

### 5.2. The main conclusions to this research are the answers to the two parts of the research question given earlier:

1. The lattice enthalpy of an ionic crystal relies on the charges of each ion and atomic radius. Ion charges has a proportional relationship regarding the lattice enthalpy, while atomic radius is inversely proportional to the strength of lattice enthalpy.

2. Generally with a higher lattice enthalpy, the melting points would be higher as well. However, some special conditions could be seen in the graph as well: In group1 metal halides, lithium halide has the lowest melting point while they have the highest lattice enthalpy; For group2 metal halides, particularly Beryllium halide has a lower melting point compared with magnesium halide while the lattice enthalpy is largest; BaCl<sub>2</sub>, BaBr<sub>2</sub>, BaI<sub>2</sub> have higher melting point than SrCl<sub>2</sub>, SrBr<sub>2</sub>, SrI<sub>2</sub> while the lattice enthalpy was lower. This difference may be caused the assumption we made regarding lattice enthalpy, assuming that all ionic crystals were in perfectly spherical form, and fully ionic characters.

## 6. Evaluation and Future work

1. Based on the research, analysis and conclusion, some interesting facts have been revealed: ionic compounds could still be more covalent since the cation distorts the electron density of the anion by Fajan's model. In this case, the ionic

crystal could be utilized in Textile Chemistry somehow under the circumstance that metals and carbon fiber have already taken part in.

2. Because many factors, such as ionic radius, ionic charges, coordination geometry, the ionic character will affect the lattice enthalpy, the relationship between the coordination geometry between the lattice enthalpy can be investigated. Also, to what extent does the ionic character can affect the lattice enthalpy and melting point can be investigated.

## References

- [1] Brown, C. , Ford, M. (2014) Higher Level Chemistry. 2nd ed. Pearson Education, Harlow, Essex.
- [2] Feng, H., Scriven, G. (2018) Accelerated Predictive Stability. Academic Press, Ridgefield, Sandwich
- [3] Encyclopedia Britannica. (2016) "melting", <https://www.britannica.com/science/melting>. Accessed 2 October 2022.
- [4] Chemistry LibreTexts. (2016) "8.9: Physical Properties of Ionic Compounds", [chem.libretexts.org/Bookshelves/Introductory\\_Chemistry/Introductory\\_Chemistry\\_\(CK-12\)/08%3A\\_Ionic\\_and\\_Metallic\\_Bonding/8.09%3A\\_Physical\\_Properties\\_of\\_Ionic\\_Compounds](https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Introductory_Chemistry_(CK-12)/08%3A_Ionic_and_Metallic_Bonding/8.09%3A_Physical_Properties_of_Ionic_Compounds).
- [5] Kurtuldu, G. , Jörg, F.L. (2020) "Multistep Crystallization and Melting Pathways in the Free - Energy Landscape of a Au-Si Eutectic Alloy." Advanced Science, vol. 7, no. 12, p. 1903544, 10.1002/adv.201903544.
- [6] Nichols, L. (2017) "6.1C: Melting Point Theory." Chemistry LibreTexts, [chem.libretexts.org/Bookshelves/Organic\\_Chemistry/Organic\\_Chemistry\\_Lab\\_Techniques\\_\(Nichols\)/06%3A\\_Miscellaneous\\_Techniques/6.01%3A\\_Melting\\_Point/6.1C%3A\\_Melting\\_Point\\_Theory](https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Organic_Chemistry_Lab_Techniques_(Nichols)/06%3A_Miscellaneous_Techniques/6.01%3A_Melting_Point/6.1C%3A_Melting_Point_Theory).

- [7] Talbot, C. , L. ,Y. (2013) . "The relationship between lattice enthalpy and melting point in magnesium and aluminium oxides." *School Science Review* 94(2013):pages. 9-11.
- [8] Ionic bonding. Ionic Bonding | Grandinetti Group. <http://www.grandinetti.org/ionic-bonding>
- [9] Search ChemSpider. ChemSpider. <https://chemspider.com/>
- [10] CHEMISTRY ATAR Course data booklet (2019), Government of Western Australia, School Curriculum and Standards Authority
- [11] Bryan, R.F. (1995), "Modern Crystallography, Vol. 2. Structure of Crystals Edited by B. K. Vainshtein, v. M. Fridkin and v. L. Indenbom." *Journal of Applied Crystallography*, vol. 28, no. 6, 1 Dec., pp. 860–860, 10.1107/s0021889895099493.
- [12] Chemical Index Database, (2020), Drug Information Express, Drug R&D, Chemical Database, site: <https://www.drugfuture.com/chemdata/>
- [13] Diploma Programme Chemistry data booklet (2007), International Baccalaureate Organization.
- [14] Chemistry Data Booklet (2013), Authority S Q. Access 3 Chemistry[J].
- [15] Chemistry Data Booklet (2013), national 5, Scottish Qualifications Authority.
- [16] Duffy, J.A. (2006) "Ionic–Covalent Character of Metal and Nonmetal Oxides." *The Journal of Physical Chemistry A*, vol. 110, no. 49, pp. 13245–13248, 10.1021/jp063846j.
- [17] Talbot, C. , Lydia, Y. (2013) "The Relationship between Lattice Enthalpy and Melting Point in Magnesium and Aluminium Oxides. Science Notes." *School Science Review*, Association for Science Education. College Lane Hatfield, Herts, AL10 9AA, UK. <Http://Www.ase.org.uk>, <https://eric.ed.gov/?id=EJ1015670>. Accessed 4 Oct. 2022.
- [18] S. L. Baldochi, I. M. Ranieri (2016), In Reference Module in Materials Science and Materials Engineering; Saleem Hashmi, Editor-in-Chief; Elsevier, Inc.: Dublin, Ireland.