#### (2989 words)

An investigation on the impact of electronegativity on experimental and theoretical lattice energies

#### Introduction

Lattice enthalpy is the energy absorbed when one mole of a solid ionic compound is separated into gaseous ions under standard conditions (Brown, 2014).

 $MX(s) \rightleftharpoons M^+(g) + X^-(g)$ 

Theoretical lattice enthalpies. Are calculated assuming the ionic crystal is made up from perfectly spherical ions with only interaction of electrostatic forces between them. The energy depends on the product of the ionic charges and the sum of the ionic radii of the ionic compound:

- An increase in the ionic radius of one of the ions decreases the attraction between the ions
- . An increase in the ionic charge increases the ionic attraction between the ions<sup>1</sup>

Theoretical lattice enthalpy for one mole is calculated with the following equation;

$$\Delta H_{lat}^{0} = \frac{R_{um}}{R_{M^{m+}} + R_{X^{m-}}}$$

This is because the interactions between ions have to be considered as a solid crystal form. Thus, the "attraction between the positive and negative ions predominates over the repulsion of ions with the same charge as ions are generally surrounded by neighbouring ions of opposite charge" <sup>2</sup>

K is a constant that depends on the geometry of the lattice and n and m are the magnitude of charges on the ions. As the ionic radii can be determined from X-ray diffraction measurements of the crystal, theoretical values can be calculated once the geometry of the solid lattice is known<sup>13</sup>.

of the solid lattice is known<sup>29</sup>. However, I have decided to use the Kapustinskii equation and modified Born-Lande equation to calculate the theoretical lattice enthalpy values because I found it difficult to measure the ion interactions of solid crystal forms to use the previous equation, \_

I used the Kapustinskii equation and modified Born-Lande equation to calculate the theoretical lattice enthalpy values

Kapustinskii equation is defined below:4

$$\Delta \mathsf{H}^{0}_{\text{lattice}} = K \cdot \frac{v \cdot |z^{+}| \cdot |z^{-}|}{r^{+} + r^{-}} \cdot \left(1 - \frac{d}{r^{+} + r^{-}}\right) \times 10^{-3}$$

 $K = 1.20200 \times 10^{-4} \text{ J m mol}^{-1}$  $d = 3.45 \times 10^{-11} \text{ m}$  $r^{+} + r^{-} = \text{sum of ionic radii (m)}$ v = number of ions in empirical formula  $z^+$ ,  $z^- =$  numeric charge of ion

Born-Lande equation is defined below:5

- 1 (Brown, 2014)
- <sup>2</sup> (Brown, 2014 ). <sup>3</sup> (Brown, 2014).
- <sup>4</sup> (Kapustinskii Equation, 2020
   <sup>5</sup> (Born-Lande Equation, 2020)

Commented [A1]: Research design, second strand: Describes the reason for selecting both equations for calculations.

$$\Delta H_{lattice} = -\frac{N_A M z^+ z^- e^2}{4\pi\epsilon_0 r_0} \left(1 - \frac{1}{n}\right)$$

- $\bullet \quad N_A = Avogadro\ constant$
- $\bullet \quad M = Madelung\ constant, relating\ to\ the\ geometry\ of\ the\ crystal$
- $z^+, z^- = numeric \ charge \ number \ of \ ion$
- $e = elementary \ charge, 1.6022 \times 10^{-19} C$
- $\epsilon_0 = permittivity \ of \ free \ space, 8.854 \times 10^{-12} C^2 J^{-1} m^{-1}$
- $r_0 = distance \ between \ ions$
- $n = Born \ exponent$  (determined experimentally by measuring the compressibility of the solid, or derived theoretically)



riablas		
ndependent variables	<ul> <li>ΔElectronegativity</li> <li>Sum of ionic radii of alkali metal and halogen</li> <li>Bond length and strength of ionic bond</li> </ul>	
Dependent variable	Absolute difference between theoretical and experimental lattice enthalpy values     Theoretical and experimental lattice enthalpy of monovalent ionic compounds	
Controlled variables	Monovalent ionic compounds formed with group 1 metals and group 7 halogens (MX lattice)     Experimental values obtained at standard condition (298, 15K and 100kPa)	Commented (A5): Research design second strand:
ethodology		Some controlled variables are identified but no information is provided on the method used to control them.
Databases	<ul> <li>a) IB chemistry data booklet (2016, Fourth edition)</li> <li>b) CRC Handbook of Chemistry and Physics</li> <li>c) Inorganic Chemistry: Principles of Structure and Reactivity</li> </ul>	
Resources	Microsoft excel	
<ul> <li>b) CRC Handbook of cl many other database</li> <li>c) Inorganic Chemistry enthalpy. Since this</li> </ul>	hemistry and Physics: contains physical data for each ion and it is commonly used for the source of es. It has been available for many years, and is cross-checked r: textbook published by Pearson Education that includes explanations and relevant data on lattice source is a tertiary source, there is possible inaccuracy of data.	Commented [A6]: Research design, second strand: The candidate uses one database and then tables where values were already selected by the authors. There will be limited data for the ionic radii. The reliability of the resources is somewhat addressed.
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difference. Therefore, I have decided to use the absolute difference values to ring the correlation. <sup>10</sup> This investigation is based on databases, so it is assumed that data is obtained in consideration of safety and ethical issues. Data collected electronically led to paper usage to be minimized., as well as saving the trees and the environment.

# Results

Table 1. Electronegativity and ionic radii of monovalent elements									
Alkali metal (Group 1)			Halogens (Group 7)						
М.	Electronegativity	lonic radii (10 <sup>-12</sup> m)	x٠	Electronegativity	lonic radii (10 <sup>-12</sup> m)				
u٠	1.0	76	F	4.0	133				
Na•	0.9	102	CI-	3.2	181				
K•	0.8	138	Br∙	3.0	196				
Rb•	0.8	152	1.	2.7	220				
Cs+	0.8	167							

Going down groups 1 and 7, ionic radii increase due to increased energy levels. Moving down groups 1 and 7, the distance between the nucleus and valence electrons increases, resulting in decreased attraction, therefore lower electronegativity value. These values are the independent variables of the ionic compounds.

#### Processed data<sup>11</sup>

IF	ΔE	Σr	BL	BS	IF	ΔE	Σr	BL	BS
LiF	3.0	209	1.5639	577	KBr	2.2	334	2.8208	380
LiCl	2.2	257	2.0207	469	кі	1.9	358	3.0478	325
LiBr	2.0	272	2.1704	418	RbF	3.2	285	2.2703	494
Lil	1.7	296	2.3919	345	RbCl	2.4	333	2.7869	428
NaF	3.1	235	1.9260	519	RbBr	2.2	348	2.9447	381
NaCl	2.3	283	2.3609	412	Rbl	1.9	372	3.1768	319
NaBr	2.1	298	2.5020	367	CsF	3.2	300	2.3454	519
Nal	1.8	322	2.7115	304	CsCl	2.4	348	2.9063	448
KF	3.2	271	2.1716	498	CsBr	2.2	363	3.0723	389
KCI	2.4	319	2.6667	433	Csl	1.9	387	3.3152	337

 $^{11}$  Refer to footnotes for the abbreviations used in the first row of the table.

**Commented [A9]: Data analysis, first strand:** The communication is precise; however, it is not clear what the source of the data is, aside from that for ionic radii.

Table 3. Lattice enthalpies<sup>12</sup>

IF	ΔH lamice at 298K (kJmol <sup>-1</sup> )							ΔA	∆%			
	т					EV						
	к	в	AV	SD	%U	в	н	AV	SD	%U		
LiF	960.4	1008.0	984.2	33.7	4.73	1049.0	1034.0	1041.5	10.6	1.43	57.3	5.50
LiCl	809.8	811.3	810.6	1.0	0.18	864.0	840.1	852.1	16.9	2.77	41.5	4.87
LiBr	772.7	766.1	769.4	4.7	0.86	820.0	781.2	800.6	27.4	4.73	31.2	3.90
Lil	717.5	708.4	713.0	6.4	1.27	764.0	718.4	741.2	32.2	5.97	28.3	3.81
NaF	872.8	902.0	887.4	20.6	3.24	930.0	914.2	922.1	11.2	1.70	34.7	3.76
NaCl	745.9	755.2	750.6	6.6	1.23	790.0	770.3	780.2	13.9	2.49	29.6	3.79
NaBr	713.3	718.8	716.1	3.9	0.76	754.0	728.4	741.2	18.1	3.40	25.1	3.39
Nal	666.6	661.2	663.9	3.8	0.81	705.0	680.7	692.9	17.2	3.45	29.0	4.18
KF	774.2	797.5	785.8	16.5	2.93	829.0	812.1	820.6	12.0	2.04	34.7	4.23
KCI	672.1	676.5	674.3	3.1	0.65	720.0	701.2	710.6	13.3	2.61	36.3	5.11
KBr	645.4	659.5	652.5	10.0	2.14	691.0	671.1	681.1	14.1	2.88	28.6	4.20
KI	606.8	623.0	614.9	11.5	2.60	650.0	632.2	641.1	12.6	2.74	26.2	4.09
RbF	741.4	761.1	751.3	13.9	2.59	795.0	780.3	787.7	10.4	1.85	36.4	4.62
RbCl	647.1	661.5	654.3	10.2	2.17	695.0	682.4	688.7	8.9	1.81	34.4	4.99
RbBr	622.3	636.4	629.4	10.0	2.21	668.0	654.0	661.0	9.9	2.10	31.6	4.79
Rbl	586.3	602.5	594.4	11.5	2.69	632.0	616.7	624.4	10.8	2.42	30.0	4.80
CsF	709.2	723.0	716.1	9.8	1.91	759.0	743.9	751.5	10.7	1.99	35.4	4.71
CsCl	622.3	622.6	622.5	0.2	0.04	670	629.7	649.9	28.5	6.01	27.4	4.21
CsBr	599.3	599.6	599.5	0.2	0.05	647	612.5	629.8	24.4	5.33	30.3	4.81
Csl	565.8	568.2	567.0	1.7	0.42	613	584.5	598.8	20.2	4.65	31.7	5.30

**Commented [A10]: Data analysis, third strand:** There is only one set of data for each value, and this limits the processing.

**Commented [A11]: Data analysis, first strand:** The processed values are difficult to follow with this type of presentation, but including the complete headings with corresponding uncertainties is challenging. Probably a landscape layout would have been more appropriate.

Commented [A12]: Data analysis, second strand: The footnotes include the uncertainties for processed values.

<sup>12</sup> IF = lonic formula

 $\Delta E$  = Electronegativity difference (±0.2)

r = Sum of radii (±2pm)

BL = Bond length (±0.0001A)

BS = Bond strength (±1kJmol')

TV= Theoretical value (±0.1kJmol')

EV= Experimental value (±0.1kJmol') K = Kapustinskii equation

B=Born-Land~ equation

AV = Average (±0.1kJmol ')

SD =Standard deviation (±0.1)

%U =Percentage uncertainty (±0.1)

1B =1B Data Booklet

H = Huheey

AA = Absolute difference (±0.1)

A% =Percentage difference (±0.1)

Database's calculation methods are not released, and although there must be some errors in each, the resources are reliable. Hence, uncertainties of each data correspond to the last decimal place of the value,									
Sample calculations Table 4. Sample calculations of Table 2 and 3									
$\begin{split} & \Delta Electronegativity \\ = (electronegativity of halogen) - (electronegativity of alkali metal) \\ & E.g. LiF 4.0 - 1.0 = 3.0 \end{split}$	Sum of ionic radii = (ionic radii of alkali metal)+ (ionicradii of halogen) E.g. LiF+ 76pm + 133pm = 209pm	Average: $=\frac{\varepsilon}{n}$ E.g. AV TV of LIF $\rightarrow \frac{960.4+1000.0}{2} = 984.2$							
Percentage difference: $\frac{(AV EV) - (AV TV)}{AV EV} \times 100\%$ E.g LiF → $\frac{1041.5 - 984.2}{1041.5} \times 100\% = 5.50\%$	Percentage uncertainty $=\frac{max \ value - min \ value}{max \ value} \times 100$ E.g. U for TV for LiF $\rightarrow \frac{1008.0 - 960.4}{1008.0} \times 100 = 4.275\%$	Range of %U = (m ax %U)- (min %U) TV 4.73% - 0.04% = 4.68% EV 6.01% - 1.43% = 4.58%							
$\Delta H^{0}_{\text{lattice}} = K \cdot \frac{v \cdot  z^{+}  \cdot  z^{-} }{r^{+} + r^{-}} \cdot \left(1 - \frac{d}{r^{+} + r^{-}}\right)$ E.g LiF $\rightarrow 1.20200 \times 10^{-4} J \cdot m \cdot mol^{-1} \cdot \frac{2!1!}{209 \times 10}$	$ \int - \times 10^{-3} \frac{-1}{1^{-12}m} \cdot \left(1 - \frac{3.45 \times 10^{-11}m}{209 \times 10^{-12}m}\right) \times 10^{-3} = 960.4 $	Absolute uncertainty = /(AV TV)-(AV EV)/ E.g. AU of LiF   984.2 - 1041.5 =57.3							

Commented [A13]: Data analysis, second strand: The candidate clarifies how the uncertainties were established. It seems as though they have been propagated.

**Commented [A14]: Data analysis, third strand:** The processing relies on limited values.

**Commented [A15]: Data analysis, first strand:** Communication of processing is not always precisee.g., units missing. At times it is unclear.

#### Evaluation of Reliability of Data

Comment on uncertainties

The data sources were evaluated by comparing the collected data. Table 3, shows a good agreement between the two average values. I calculated the absolute difference as uncertainty value. 4.68% and 4.58% of the percentage uncertainty range indicate the values are close to the average values. Thus, results are reliable and can be used to show a correlation in lattice enthalpies of each ionic compound,

#### Analysis and conclusion



<sup>13</sup> Error bars are not included in Figure 2 because it would be skewed by the scattered values.

Commented [A16]: Data analysis, second strand: Considers impact of uncertainties.

Commented [A17]: Data analysis, third strand: The outlier for average experimental data is not identified. The trendline chosen for this set does not look like the best choice. The candidate includes the equations for the functions.

Commented [A18]: Data analysis, second strand:  $\mathsf{R}^2$  values are reported.

results are justified to some extent.

Figure 2, shows that as the sum of ionic radii of metal and halogen ions increases, the lattice enthalpy decreases. As the distance increases, the attraction between them will decrease, as the nuclei are further apart, and less energy is required to break one mole of solid ionic compound to form gaseous ions (decrease in lattice enthalpies). The negative relationship is not linear, and appears to be steeper at lower sum of radii and the same increase in distance between two nuclei has less effect as the distance increases.

Initially, the decrease is more significant than the same decrease in the ionic radii when the radius is doubled. The gap between theoretical and experimental values seems to narrow down as sum of ionic radii increases, suggesting that very large ionic radii would have smaller differences. The differences would be minimized only if the sum of radii value is very high and there would be still considerable differences between the TV and EV even if the sum of ionic radii is 0.

Uncertainties of ionic radii are within 5 % as radii values are too small. Data are significant and errors are too small to be observed. Assuming that error bar values are uncertainty values of each TV and EV, the biggest error bar would be with LiF (46.6) for TV, and CSCI (39.1) for EV. Overall, the sum of ionic radii of monovalent ionic compounds as a factor of determinant of electronegativity may contribute to change in the gap between theoretical and experimental lattice <u>ienthalpies</u>.



Commented [A20]: Conclusion, first strand: The report considers the impact of the uncertainties on the results. Commented [A21]: Data analysis, second strand: Lines are of best fit. Outliers have not been identified.

Commented [A19]: Conclusion, second strand: The

Data analysis, third strand: The trendline that has been chosen for both averages does not look like the most adequate.

Figure 3 shows that the average theoretical lattice enthalpy values of ionic compounds are constantly higher than the corresponding average experimental lattice enthalpy values. The gradients of two trend lines are similar and the distance of theexponential equations are only 48.4 [apart]. There is a pattern in ionic bond length and lattice enthalpies as the theoretical and experimental values tend to decrease at the same rate. This may result from the relationship between ionic bond length and the electrostatic forces of ionic compounds, suggesting that ionic bond length has a negative correlation with lattice enthalpy values, increasing  $\Delta$ Electronegativity of ionic compounds.

I measured the sum of ionic radii and bond length despite those having approximately the same values, because the "ionic character of a bond depends on the strength of the force holding ions in lattice. Hence, the stronger the force of attraction, the greater the lattice enthalpy"<sup>44</sup> Ionic radii only take account of ionic character, so I compared ionic bond lengths to attempt identifying new relationships in theoretical lattice enthalpies which are considered to exclude any ionic characters.

Uncertainties are within 5% indicating that values are significant with high reliability. Overall, decreasing trend in ionic bond length corresponding to lattice enthalpies suggests that electronegativity values may cause change in the difference between theoretical and experimental lattice enthalpies.

<sup>14</sup> (Brown, 2014).

Commented [A22]: Conclusion, first strand: It is unclear which is the distance the candidate recurrently uses in the analysis. Uncertainties are considered.





I plotted another diagram using experimental lattice enthalpy values as dependent variables to take ionic characters into account. There were positive trends as moving down the group 7, and regarding group 1, there is a slight decrease in the gradients of linear regression lines. This suggests that although there is the same increase in bond strength of Li, there will be a slight difference in that of CsX. This may be due to the size of difference in between group 1 which can affect the bond strength and lattice enthalpies.



I plotted values moving down the group such as MF, MCI MBr, and MI<sup>1</sup>. There were generally decreasing trends, except for MF series. This may be due to the small size of Fluoride affecting both bond strengths and experimental lattice enthalpies.

There was no clear pattern in the gradients, especially for MF compounds, as values don't decrease as you move down the group 7. MF compounds exhibit higher lattice enthalpy values than other compounds. We can state that increasing size of the halogen corresponds with lower lattice enthalpy. Moving down group 1, lattice enthalpy decreases. Despite not consistent trends in metal halogen ionic compounds, I may state that there is a general negative trend observed in increasing bond strength and experimental lattice enthalpy moving down group 1 metals. The ionic compounds tend to exhibit general trends moving down group 1 metals and group 7 halogens, although there is not a clear correlation between bond strength and electronegativity.

3. Effect of ΔElectronegativity<sup>15</sup>

**Commented [A27]: Conclusion, first strand:** Five values are needed for establishing a trend and the trendlines show extremely weak correlations. The candidate identifies this issue.



This graph summarizes the effect of factors affecting electronegativity values and answers my hypothesis. Due to minimal uncertainties of the absolute difference between theoretical and experimental lattice enthalpy (±0.1), y-value error bars are not observed.

The result goes against my hypothesis. There is a weak correlation and we can observe few data not following the trend, especially\_ LIF compounds. This indicates that there is not really a close relationship between those variables, probably due to procedural errors in enthalpy measurement, such as heat loss from the system or possible pressures of the gases involved (Jason, 2017).



As in Figure 7, there is a slight increase in  $r^2$  value (0.3039), but the value is too low, and there is not much relationship between  $\Delta E$ and  $\Delta A$ . Overall, I can conclude that there is no relationship between electronegativity difference and the difference between theoretical and experimental lattice enthalpies.

In brief:

- 1) The sum of ionic radii, bond length, and bond strength of ionic compounds formed from alkali metals and halogens show higher lattice enthalpies on theoretical values than experimental values. This is because those affect electronegativity values in ionic compounds that can affect the difference between theoretical and experimental lattice enthalpies. The relationships in sum of ionic radii and bond length were relatively stronger than that of bond strength. Instead, there were trends related to periodic characters observed in the relationship with bond strength.
- 2) The effect of electronegativity differences of ionic compounds on changes of difference in theoretical and experimental lattice enthalpies is inconsiderable. As the electronegativity increases the change in difference between theoretical and experimental lattice enthalpy is less responsive in terms of covalent character of ionic compounds.

**Commented [A28]: Conclusion, first strand:** With the very low correlation coefficient the candidate has no solid evidence supporting the claim of a weak correlation.

**Commented [A29]: Data analysis, second strand:** The candidate identifies the outlier but excludes it without any justification.

Commented [A30]: Conclusion, second strand: There is a very limited use of pertinent theory. There is no consideration of the theoretical model. Experimental data suggest a combination of ionic forces and some additional covalent character in the bonding model. The conclusion contradicts the accepted scientific context. Polarizing effects of small ions are ignored. My hypothesis was partially refuted. Extra conditions should be also considered in order to obtain a clear correlation between\_ ΔElectronegativity and the difference between theoretical and experimental lattice enthalpies.

Evaluation

**Commented [A31]: Evaluation, second strand:** The candidate offers no clarifications on extra conditions, resulting in no real improvement being stated.

Limitation	Significance	Improvement		
Different methods of measuring experimental data	The difficulties in controlling heat loss andstandard conditions might have contributed to further inaccuracy of data (systematic error).	It would be better to use data from one specific database that has a uniformed method of obtaining experimental data. This would reduce the variance in experimental data and increase		Commented [A32]: Eva
		the reliability of obtained data.		improvement is explaine contradicted by another
Uncertainty values from _ each database	As uncertainty values are not mentioned from the databases that I used, it is difficult to calculate exact uncertainty values, lowering the reliability of data	Finding the primary source of data is essential to calculate the exact uncertainty values from each database. As major uncertainty values come from volumetric apparatus, the exact		Commented [A34]: Eva valid limitation and it is r
	Teliability of data.	methodology for each database can be found and applied in uncertainty calculation		
Exclusion of ionic	I have excluded ionic compounds that are not	Comparing the values and trends of other		improvement is explained
compounds that are not formed with alkali metals	formed with group 1 and group 7 from my investigation although these are monovalent	monovalent ionic compounds that are not formed with alkali metals and halogens with the		
and halogens	_ionic compounds due to unobtainable data. For example, adding AgX compounds to investigation would have showndifferences in electropeativity. Jeading to different	values   found in this investigation would lead to more thorough and depth study. This can make me understand the reason behind some of the extreme values and the weak relationship		Commented [A36]: Eva valid limitation to be exp covering 10 hours. The
	conclusions that what I have got.	between electronegativity differenceand the difference between theoretical and experimental		
Subjective selection of collected data	As I mainly collected my data from 1B Chemistry data booklet and CRC Handbook of Chemistry and Physics, there might be possible inaccuracy on percentage difference derived from each source used to obtain lattice enthalpies.	lattice enthalpies		<b>Commented [A37]: Eva</b> allocation of time for this a realistic improvement.
				Commented [A38]: Eva method for selecting the justified.
			<u> </u>	<b>Commented [A39]: Eva</b> Explains a realistic impro previous suggestion for
Lack in representation of reality	Experimental lattice enthalpies are obtained via Born-Haber cycles and require long series of steps. Theoretical lattice enthalpies might be approximate value instead of the exact value.	It is only possible toreduce the errors found in experimental lattice enthalpies, but not realistic at school level.		
	which may lack representation of reality			<b>Commented [A40]: Eva</b> remains unclear if the ca understanding of the diff and theoretical values.

**Commented [A32]: Evaluation, first strand:** This is a valid limitation, and it is explained to some extent.

Commented [A33]: Evaluation, second strand: The mprovement is explained. However, it is later contradicted by another suggested improvement.

Commented [A34]: Evaluation, first strand: This is a valid limitation and it is reasonably explained.

**Commented [A35]: Evaluation, second strand:** The improvement is explained, but is not realistic.

**Commented [A36]: Evaluation, first strand:** This is a valid limitation to be expected in an investigation covering 10 hours. The explanation is reasonable.

Commented [A37]: Evaluation, second strand: The allocation of time for this component does not make this a realistic improvement.

Commented [A38]: Evaluation, first strand: The method for selecting the data is not explained or ustified

**Commented [A39]: Evaluation, second strand:** Explains a realistic improvement but contradicts a previous suggestion for improvement.

Commented [A40]: Evaluation, first strand: It remains unclear if the candidate has a clear understanding of the differences between experimental and theoretical values.

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