The Effect of Branching on Enthalpy of Formation of Alkanes

1 Introduction

The standard enthalpy of formation $\Delta H_f^{\ominus}$ of a compound gives the enthalpy change that occurs when one mole of a particular substance is formed from its elements in their standard states (Brown and Ford 228). Chemicals tend to react in a way that leads to lower stored energy in the products, leading to greater stability compared to the reactants. As such, the standard enthalpy of formation $\Delta H_f^{\ominus}$ is an important measure of its thermodynamic stability relative to its elements. However, consider the following reaction giving the formation of Butane:

$$4\,\mathrm{C}_{(\mathrm{graphite})} + 5\,\mathrm{H}_{2(\mathrm{g})} \longrightarrow \mathrm{C}_4\mathrm{H}_{10(\mathrm{g})} \tag{1.1}$$

When attempting to calculate the $\Delta H_f^{\ominus}$ for this formation reaction, I noticed that using bond enthalpy calculations would only give a single value, even though there are two possible structural isomers for C_4H_{10}, n-Butane and 2-methylpropane.

Furthermore, when learning about using bond enthalpies to calculate enthalpies of formation, it was emphasized that the bond enthalpies provided in the IB Data Booklet are only the “average” values and the actual values in fact are dependent on their environment (231). This had me wondering about how the structural isomerism on alkanes might affect bond enthalpies and the enthalpies of formation of various alkane isomers. This leads us to the research question of this investigation:

> *How does the extent of branching in structural isomers of a particular alkane affect their stability?*

2 Hypothesis

In highly branched alkanes, it is possible that electron clouds of the branches being close to one another can introduce internal steric repulsion. This can result in increased instability. The hypothesis is that this effect will get more pronounced the closer the branches are to the centre of the molecule as there is stronger such steric repulsion. Hence, the enthalpy of formation is expected to increase (i.e., less negative) for increasingly branched alkanes. It is also expected that the magnitude of the enthalpy of formation decreases as the branching point is closer to the centre.

3 Methodology

Independent Variable: Extent of Branching

It is not immediately obvious how the extent of branching can be rigorously quantified. In this investigation, factors that could be considered as part of "amount of branching" such as the length and position of individual branches were ignored in favour of a simpler approach to quantify branching – the number of endpoints. In the case of alkanes, endpoints are always CH_3 groups. Hence, the extent of branching in this paper will be quantified by the number of CH_3 groups present in a molecule. An additional reason to use this approach of quantifying branching is because this automatically corresponds to two more than the number of branches suggested by the IUPAC naming convention. Consider the isomers of Pentane in Figure 1 as an example. Red circles are used to identify CH_3 groups (”endpoints”). The number of endpoints in Pentane is 2, in 2-methyl Butane is 3, and Neopentane is 4.

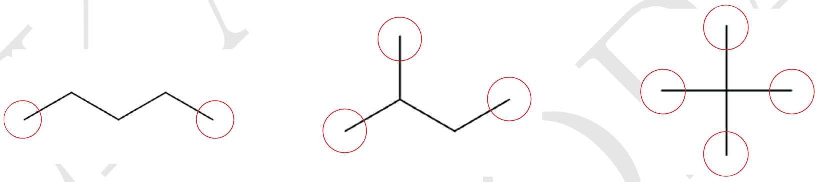
(a) Pentane (b) 2-methyl Butane (c) Neopentae

Figure 1. Endpoints in Isomers of Pentane. Images made with Adobe Illustrator and MolView by Bergwerf.

Dependent Variable: Gas Phase Enthalpy of Formation (ΔH_f°)

Control Variables:

1. Only alkanes are being considered so all bonds that could affect the data are single, sigma bonds.
2. All enthalpy of formation data is obtained for standard states at standard temperature (298.15 K) and standard pressure (1 atm)

To determine the presence of any correlations, the enthalpy of formation, ΔH_f° is plotted against the number of CH_3 groups for alkanes with a certain number of carbon atoms. This is then repeated for alkanes with different number of carbon atoms. Data for alkanes from C_4H_{10} to C_8H_{18} is used. This range is used primarily because of the availability of multiple sources of enthalpy of formation data for all possible isomers of the alkanes. Such data is scarce for alkanes with more Carbon atoms than C_8H_{18}. Alkanes with fewer Carbon atoms than C_4H_{10} do not form isomers.

The following databases have been used in the data collection:

1. NIST Chemistry WebBook (Afeefy et al.)

The NIST Chemistry WebBook was chosen for several reasons. Firstly, it is a highly authentic resource given its status as a United States government initiative. Secondly, it is easy to use as data can be obtained for all isomers of a certain alkane just by searching a particular chemical formula. Thirdly, it contains notes and references for all the data. This makes it very suitable for evaluation especially with the explicit uncertainty values provided. It must be noted that the NIST WebBook only compiles data. To remain consistent, only data collectively attributed to Prosen and Rossini was used for this investigation (with the exception of the data for Butane isomers which was attributed to Maron alongside Prosen and Rossini). Data from this source was given in kJ/mol to a precision of 1 decimal place. Uncertainty information varied between 1 and 2 decimal places.

2. American Institute of Physics Handbook (Gray)

   The American Institute of Physics is a reputed organisation, lending to the reliability of the data in this Handbook. This resource also contains explicit uncertainty information for evaluation. In addition, it is freely available for free on MIT's website. Data in this source was given in kcal/mol to a precision of 2 decimal places or 4 significant figures. A conversion factor was provided which was used to convert the data to kJ/mol to a precision of 4 significant figures . Explicit individual uncertainty values were not given. Instead, a range of uncertainty was given for the entire dataset. The midpoint of this range converted to kJ/mol and corrected to 1 significant figure was used.

3. Thermochemical Data of Organic Compounds (Pedley et al.)

   This is a dataset collected by scientists at the University of Sussex. The methodology through which the data was obtained was explained in detail, making it possible to evaluate the reliability of the data. This is also the database with the newest data among these three. Hence newer, more accurate and precise methods may have been used to obtain the data. Data in this source was given in kJ/mol to a precision of 1 decimal place. Uncertainty information was given to a precision of 1 decimal place.

There are no safety and ethical considerations in this paper as all data was obtained from pre-existing databases where experiments were already conducted.

As can be noted from the data in tables 3, 4 and 5 in the appendix, all three sources have data almost always within range of 3 kJ/mol of each other. Due to the consistency in the data across the three sources, no values had to be discarded due to being outliers.

4 Data Processing

To process the data, first the enthalpy of formation data for each isomer was averaged between the three databases. Uncertainties were obtained by taking half of the range of data and correcting it to the lowest number of significant figures involved in the calculation. In this case since the uncertainties for the American Institute of Physics Handbook data were all 1 significant figure, the average uncertainties were also corrected to 1 significant figure.

Table 1. Averaged Data from the three Data Sources

Number of Endpoints	Number of Carbon Atoms									
	4		5		6		7		8	
	Isomer	$\Delta H_f^{\ominus}$ (kJ/mol)	Isomer	$\Delta H_f^{\ominus}$ (kJ/mol)	Isomer	$\Delta H_f^{\ominus}$ (kJ/mol)	Isomer	$\Delta H_f^{\ominus}$ (kJ/mol)	Isomer	$\Delta H_f^{\ominus}$ (kJ/mol)
2	n-Butane	-126.3 ± 1	n-Pentane	-146.6 ± 1	n-Hexane	-167.1 ± 1	n-Heptane	-187.7 ± 1	n-Octane	-208.4 ± 1
3	2-methyl Propane	-134.8 ± 1	2-methyl Butane	-154.2 ± 1	2-methyl Pentane	-174.4 ± 1	2-methyl Hexane	-194.8 ± 1	2-methyl heptane	-215.4 ± 1
							3-methyl Hexane	-191.9 ± 2	3-methyl Heptane	-212.5 ± 1
					3-methyl Pentane	-171.7 ± 1	3-ethyl Pentane	-189.6 ± 1	4-methyl Heptane	-212.0 ± 1
									3-ethyl Hexane	-210.8 ± 1
4	-	-	Neopentane	-166.7 ± 2	2,2-dimethyl Butane	-185.7 ± 1	2,2-dimethyl Pentane	-206.1 ± 2	2,2-dimethyl Hexane	-224.6 ± 1
									2,3-dimethyl Hexane	-213.8 ± 2
							2,3-dimethyl Pentane	-198.0 ± 3	2,4-dimethyl Hexane	-219.3 ± 1
									2,5-dimethyl Hexane	-222.5 ± 2
					2,3-dimethyl Butane	-178.0 ± 1	2,4-dimethyl Pentane	-201.9 ± 1	3,3-dimethyl Hexane	-220 ± 1
									3,4-dimethyl Hexane	-212.9 ± 2
							3,3-dimethyl Pentane	-201.3 ± 1	2-methyl-3-ethyl Pentane	-211.1 ± 1
									3-methyl-3-ethyl Pentane	-214.9 ± 1
5	-	-	-	-	-	-	2,2,3-trimethyl Butane	-204.7 ± 1	2,2,3-trimethyl Pentane	-220.0 ± 2
									2,2,4-trimethyl Pentane	-224.1 ± 2
									2,3,3-trimethyl Pentane	-216.3 ± 2
									2,3,4-trimethyl Pentane	-217.3 ± 2
6	-	-	-	-	-	-	-	-	2,2,3,3-tetramethyl Butane	-225.8 ± 2

After this, the mean $\Delta H_f^\ominus$ for alkanes with the same number of carbon atoms and same number of endpoints were calculated. Due to outliers, using the median instead was initially considered. However, the average was used in the end as it would take in account the effect of all isomers with a certain number of endpoints, making any visible trends more generally applicable and not skewed to the data that fits. As these mean $\Delta H_f^\ominus$ values are calculated from measurements of different isomers and not multiple measurements of the same isomer, uncertainties do not apply in a conventional sense. Hence, to ascertain if a correlation generally exists, the minimum and maximum $\Delta H_f^\ominus$ among alkanes with the same number of carbon atoms and same number of endpoints are also considered in addition to the statistical mean. The minimum and maximum values used take into account uncertainty (i.e., the uncertainties are added to the measured values before choosing the maximum and subtracted before choosing the minimum). Note that the magnitudes of maximum values are smaller than the magnitude of minimum values; this is because the $\Delta H_f^\ominus$ for all alkanes is negative.

These mean, maximum and minimum values were tabulated for alkanes with different numbers of endpoints and carbon atoms:

Table 2. Mean, Minimum and Maximum $\Delta H_f^\ominus$ for Isomeric Alkanes with a Fixed Number of Endpoints

Number of Carbon Atoms	Number of Endpoints	Mean $\Delta H_f^\ominus$ (kJ/mol)	Maximum $\Delta H_f^\ominus$ (kJ/mol)	Minimum $\Delta H_f^\ominus$ (kJ/mol)
4	2	-126.3	-125.3	-127.3
4	3	-134.8	-133.8	-135.8
5	2	-146.6	-145.6	-147.6
5	3	-154.2	-153.2	-155.2
5	4	-166.7	-164.7	-168.7
6	2	-167.1	-166.1	-168.1
6	3	-173.1	-170.7	-175.4
6	4	-181.9	-177	-186.7
7	2	-187.7	-186.7	-188.7
7	3	-192.1	-188.6	-195.8
7	4	-201.8	-195	-208.1
7	5	-204.7	-203.7	-205.7
8	2	-208.4	-207.4	-209.4
8	3	-212.7	-209.8	-216.4

8	4	-217.4	-210.1	-225.6
8	5	-219.4	-214.3	-226.1
8	6	-225.8	-223.8	-227.8

5 Analysis

The graphs below plot the mean, minimum and maximum ΔH_f° against endpoints for isomers of alkanes with a specific number of carbon atoms. Note that there are no error bars for these graphs, since these are statistical values and not individual, measured data points. In some sense, the use of the statistical minimum and maximum values corresponds to the use of error bars in a conventional measured data.

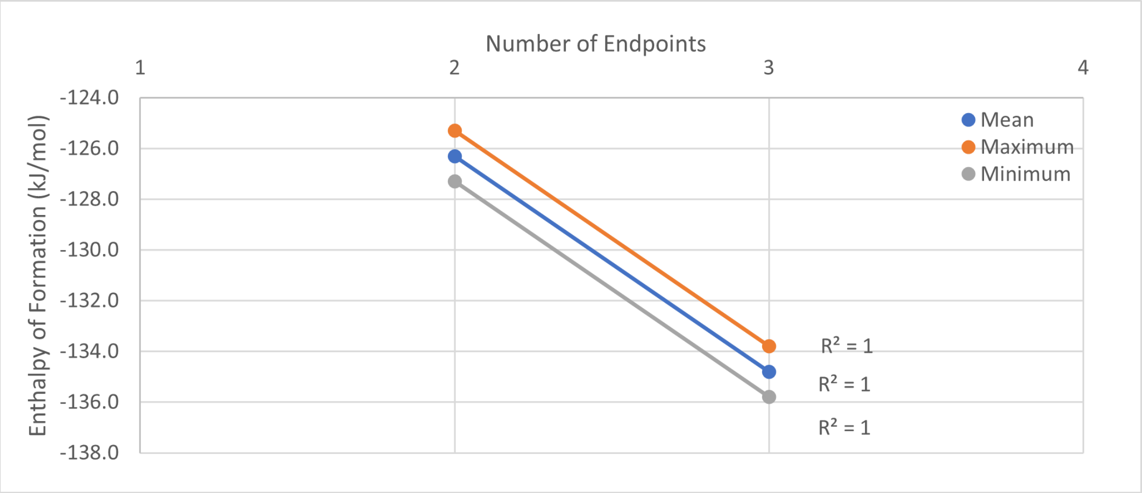

Figure 2. ΔH_f° (kJ/mol) plotted against Number of Endpoints for isomers of Butane.

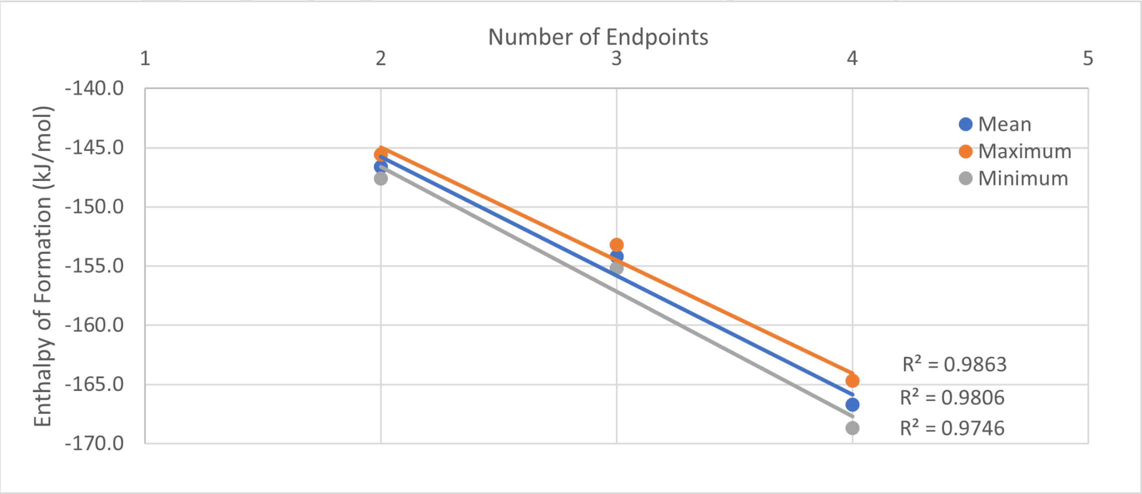

Figure 3. ΔH_f° (kJ/mol) plotted against Number of Endpoints for isomers of Pentane.

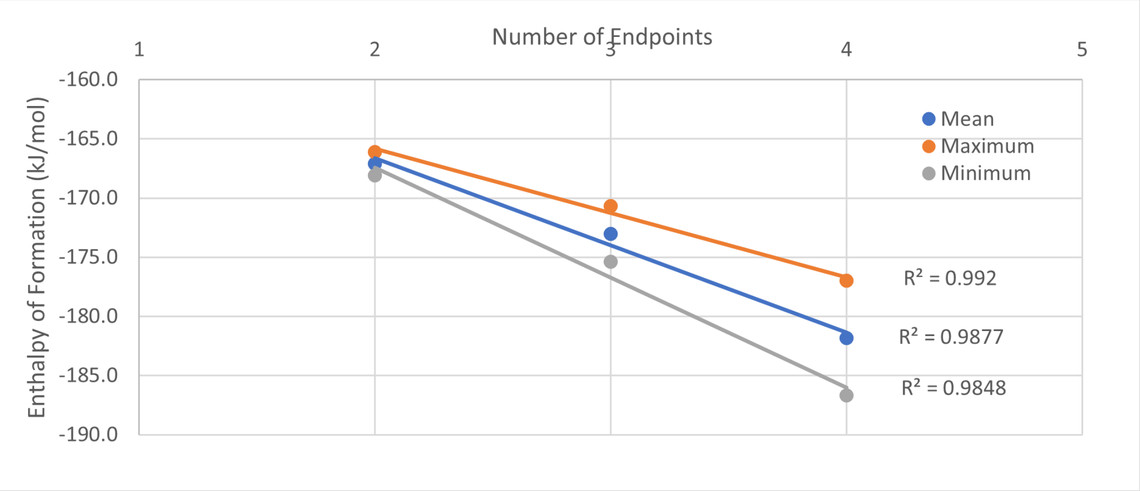

Figure 4. ΔH_f° (kJ/mol) plotted against Number of Endpoints for isomers of Hexane.

The above 3 graphs suggest a negative correlation between branching and the ΔH_f°. This correlation is consistent across all cases, for the mean, minimum and maximum. Interestingly, this result contradicts the initial hypothesis that branching would cause the enthalpy of formation to increase. Instead, this trend suggests that branching causes a decrease in the ΔH_f°, implying branched alkanes are more stable than linear alkanes.

Note that for the above three graphs, due to the presence of only two to three data points, the nature of this correlation (i.e., whether it linear or inverse exponential etc.) cannot be confidently determined. Hence, the R^2 values generated by Microsoft Excel have been ignored.

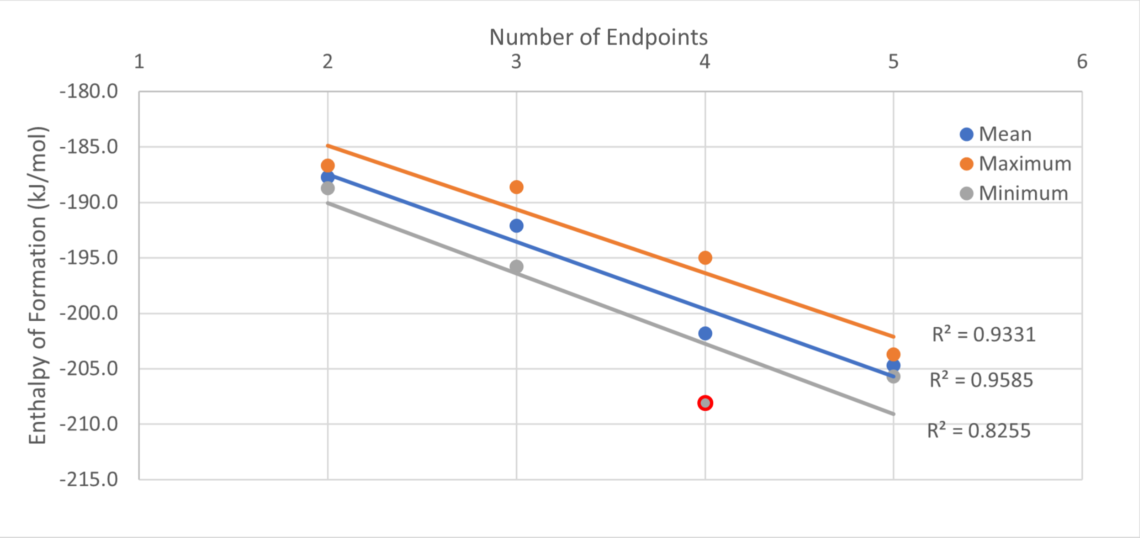

Figure 5. ΔH_f° (kJ/mol) plotted against Number of Endpoints for isomers of Heptane.

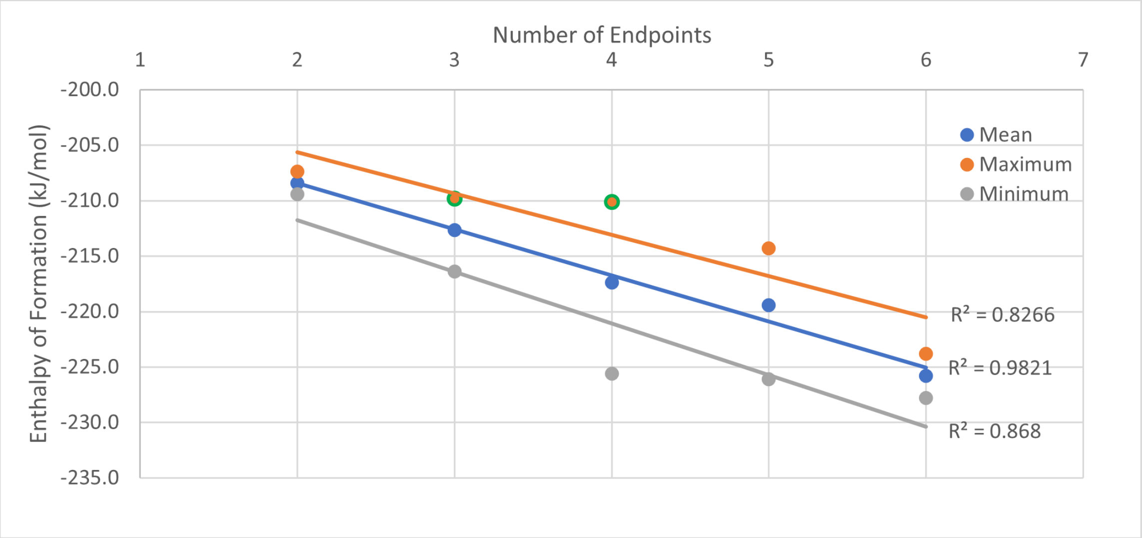

Figure 6. ΔH_f° (kJ/mol) plotted against Number of Endpoints for isomers of Octane.

The above two graphs generally agree with the overall negative correlation seen earlier. In the case of the mean ΔH_f°, both graphs show a linear relationship with $R^2 > 0.95$. However, for the minimum and maximum graphs, there are a few values that do not perfectly align with the trend. For example, the maximum ΔH_f° values for isomers of octane with 3 and 4 endpoints, outlined green in graph 5, are almost equal. Nonetheless, the value for 4 endpoints is still lower than the value with 3 endpoints, in line with the negative correlation.

However, there is one major outlier, outlined in red in figure 5. The minimum value for isomers of heptane with 4 endpoints is lower than the minimum value for 5 endpoints. Looking back at the values from table 1, we can see that this is due to 2,2-dimethylpentane having an ΔH_f° that is more negative than that of 2,2,3-trimethylbutane. This implies that the number of branches is not the only factor in alkane stability.

An interesting pattern we can observe is that alkanes with two methyl branches at the 2,2 positions tend to have significantly more negative ΔH_f° values compared to all of their other isomers with four endpoints. For example, 2,2-dimethyl Hexane has the most negative ΔH_f° amongst isomers of Octane with 4 endpoints and 2,2-dimethyl Butane has the most negative ΔH_f° amongst isomers of Hexane with 4 endpoints. This may also be the reason for the comparable values of minimum ΔH_f° between 4 and 5 endpoints for isomers of Octane. This observation suggests that the positions and lengths of the branches also have a role in the stability of alkanes.

Overall, aside from a few irregularities, a consistent negative correlation is observed between ΔH_f° and the number of endpoints for isomers of a certain alkane. This correlation is observed in the mean, minimum and maximum case. In the mean case, this correlation is appreciably linear. In response to the research question - “How does the number of branches in structural isomers of a particular alkane affect their stability?" - this leads to the conclusion that an increase in branching leads to a more negative enthalpy of formation, and hence an increase in stability.

6 Discussion

As noted earlier, the above conclusion confirms that the data contradicts the initial hypothesis. It is not evident from these results why such a relationship exists. However, it is clear that branching either does not lead to internal steric repulsion or any internal steric repulsion produced is offset by unknown stabilising interactions responsible for this behaviour. Existing research about what these stabilizing interactions could be is inconclusive.

Pitzer and Catalano, who in 1956 published some of the earliest research on this matter, proposed an "electron correlation effect" which is described as an attractive intramolecular London Dispersion Force (Pitzer and Catalano 4844). Branched alkanes were proposed to have greater intramolecular attraction between non-bonded atoms than linear alkanes and were hence seen to be more stable. However, Bartell dispelled this theory in 1960 when he observed that Pitzer and Catalano's research ignored repulsive nonbonded interactions that were shown to come into play at such short intramolecular distances (Bartell 828). Much later in 2005, Gronert writes, "The key issue is that Pitzer's argument depends on exceedingly large van der Waals attractions, which can only be attained at very short distances, but these distances are deep into the repulsive portion of a molecular interaction surface" (Gronert, "An Alternative Interpretation of the C—H Bond Strengths of Alkanes" 1216).

In the same paper, Gronert presents an alternative explanation for this relation. He posits that 1,3 repulsive interactions between non-bonded atoms are instead key factors in the stability of hydrocarbons. He terms these "geminal interactions". In the context of saturated hydrocarbons, there are three such geminal interactions possible: C-C-C, H-C-C and H-C-H.

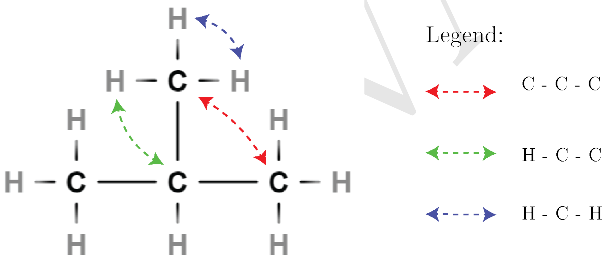

Figure 7. Examples of the Types of Geminal Repulsions Present in Isobutane. Images made with Adobe Illustrator and MolView by Bergwerf.

These repulsions are due to similar reasons to above – the distances between 1, 3 atoms are smaller than their van der Waals radii should be. Gronert finds that the repulsion between H-C-H interactions is significantly smaller than that between H-C-C and C-C-C interactions. Observing that each additional branch (such that the total number of carbon atoms in the alkane remains the same) replaces 2 H-C-C interactions with 1 weaker H-C-H interaction and 1 C-C-C interaction, Gronert concludes that branched isomers have less overall geminal repulsion and hence are more stable molecules.

Not long after, Wodrich and Schleyer publish findings that a model involving only 1 attractive term instead of 3 repulsive ones can also achieve similarly accurate estimates of ΔH_f° values (Wodrich and Schleyer 2137). They argue that Gronert's findings are correlative rather than causal. Wodrich and Schleyer conjecture in their work that 1,3 C-C-C interactions are not repulsive, but stabilizing. In a subsequent paper, they term this stabilizing interaction "protobranching" (Wodrich et al. 7731). As a consequence, highly branched alkanes which have more C-C-C interactions than alkanes with lesser branching, tend to be more stable. However, while they evaluate this concept based on empirical calculations, no physical explanation for the net attractive nature of this interaction was given. This was a point Gronert heavily argued in a correspondence (Gronert, "The Folly of Protobranching" 5375).

The latest research continues on the protobranching line, though no consensus appears to have been reached. It is a testament to the evolving nature of science that this seemingly simple question that even high schoolers like myself can explore has been under scrutiny by scientists for upwards of 80 years and still has no agreed upon answer. In my view, Gronert's geminal repulsion hypothesis is more convincing as it is not only accurate at predicting enthalpies of formation but the source of this repulsion has also been clearly identified. Until a source of protobranching attraction interaction is determined, this hypothesis stands as a purely mathematical.

7 Evaluation

Key Methodological Choices/Limitations	**Impact**	**Future Work**
Limited data from only alkanes ranging between 4 to 8 carbon atoms was used.	This was mostly due to the limited availability of data. It is possible that large, extensively branched alkanes exhibit stabilities that do not agree with the correlation observed here.	Since gaseous state enthalpy of formation data was not available for all isomers of alkanes with more than 8 carbon atoms, other methods of measuring stability such as those mentioned below could be used in future investigations.

The amount of branching was quantified with the number of endpoints (the number of -CH3 groups).	This approach treats all alkanes with the same number of endpoints equally even though they may be branching from distinct positions and have different numbers of carbon atoms which might affect stability. Nonetheless, the effects of this simplification were mitigated as much as possible through the consideration of minimum and maximum values to consider all extremes of the data in finding a correlation. Ultimately, a clear trend is still obtained. However, this method does not allow us to draw conclusions about the reason for such a correlation.	While this investigation focuses on only the number of branches, the surface areas or volumes of different isomers could have been a possible approach to quantify the overall effect of branching on different alkanes. It is a measurable quantity that considers the effect of branch length and position as well as the number of branches. Isomers with the same number of endpoints would have unique values for surface area and volume, leading to more data points. However, obtaining values for these surface areas and volumes proved difficult and would be more feasible with access to paid, professional software and databases.
None of these databases make any mention about the conformation of the alkanes from which the data was obtained.	Since the variation in enthalpy of formation across the different isomers is small, the conformation of the alkanes from which the data was obtained could have significant effects on the correlations observed. It is reasonable to assume that the data was obtained from the most stable conformation of each alkane since those are what are most found.	The methodology behind how the data from each of the isomers should be reviewed carefully to ensure alternative conformations do not have a significant effect on enthalpy of formation data.

The choice to quantify stability based on enthalpy of formation	In this investigation, stability was quantified with enthalpy of formation values. This is not the only way to do this. For example, enthalpy of combustion data can also be used, where alkanes with lower enthalpies of combustion are more thermodynamically stable. It should be noted that enthalpy of formation is a relative measure of stability in comparison to the standard states. Since all the isomers are alkanes consisting only of carbon and hydrogen atoms, this is a suitable way of comparing stability.	Subsequent investigation could make use of enthalpy of combustion data or Gibb's free energy of formation to determine if a corresponding correlation is observed.

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A Appendix

Table 3. **Raw Data from NIST Chemistry Web Book**

Number of Endpoints	**Number of Carbon Atoms**									
	4		5		6		7		8	
	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)
2	n-Butane	-127.1 ± 0.67	n-Pentane	-146.4 ± 0.67	n-Hexane	-167.2 ± 0.79	n-Heptane	-187.8 ± 0.79	n-Octane	-208.4 ± 0.67
3	2-methyl Propane	-135.6 ± 0.54	2-methyl Butane	-154.5 ± 0.84	2-methyl Pentane	-174.3 ± 1.0	2-methyl Hexane	-195.0 ± 1.3	2-methyl heptane	-215.5 ± 1.3
							3-methyl Hexane	-192.3 ± 1.3	3-methyl heptane	-212.6 ± 1.1
					3-methyl Pentane	-171.6 ± 0.96	3-ethyl Pentane	-189.7 ± 1.2	4-methyl heptane	-212.1 ± 1.2
									3-Ethyl hexane	210.9 ± 1.2
4	-	-	Neopentane	-166.0 ± 1.0	2,2-dimethyl Butane	-185.6 ± 0.96	2,2-dimethyl Pentane	-206.2 ± 1.3	2,2-Dimethyl hexane	-224.7 ± 1.0
									2,3-Dimethyl hexane	-213.9 ± 1.5
							2,3-dimethyl Pentane	-199.2 ± 1.3	2,4-Dimethyl hexane	-219.4 ± 1.1
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					2,3-dimethyl Butane	-177.8 ± 1.0	2,4-dimethyl Pentane	-202.1 ± 0.96	3,3-Dimethyl hexane	-220.1 ± 1.1
									3,4-Dimethyl hexane	-213.0 ± 1.5
							3,3-dimethyl Pentane	-201.5 ± 0.92	2-methyl-3-ethyl pentane	-211.2 ± 1.3
									3-methyl-3-ethyl pentane	-215.0 ± 1.3
5	-	-	-	-	-	-	2,2,3-trimethyl Butane	-204.8 ± 1.1	2,2,3-Trimethyl pentane	-220.1 ± 1.5
									2,2,4-Trimethyl pentane	-224.1 ± 1.3
									2,3,3-Trimethyl pentane	-216.4 ± 1.4
									2,3,4-Trimethyl pentane	-217.4 ± 1.7
6	-	-	-	-	-	-	-	-	2,2,3,3-Tetramethyl butane	-225.9 ± 1.9

Table 4. **Raw Data from American Institute of Physics Handbook**

Number of Endpoints	Number of Carbon Atoms									
	4		5		6		7		8	
	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)
2	n-Butane	-126.1 ± 0.9	n-Pentane	-146.4 ± 0.9	n-Hexane	-167.0 ± 0.9	n-Heptane	-187.7 ± 0.9	n-Octane	-208.3 ± 0.9
3	2-methyl Propane	-134.5 ± 0.9	2-methyl Butane	-154.4 ± 0.9	2-methyl Pentane	-174.1 ± 0.9	2-methyl Hexane	-194.8 ± 0.9	2-methyl heptane	-215.4 ± 0.9
							3-methyl Hexane	-192.1 ± 0.9	3-methyl heptane	-212.5 ± 0.9
					3-methyl Pentane	-171.5 ± 0.9	3-ethyl Pentane	-189.5± 0.9	4-methyl heptane	-211.7 ± 0.9
									3-Ethyl hexane	-210.7 ± 0.9
4	-	-	Neopentane	-165.9 ± 0.9	2,2-dimethyl Butane	-185.4 ± 0.9	2,2-dimethyl Pentane	-206.1 ± 0.9	2,2-Dimethyl hexane	-224.6 ± 0.9
									2,3-Dimethyl hexane	-213.8 ± 0.9
							2,3-dimethyl Pentane	-195.7 ± 0.9	2,4-Dimethyl hexane	-219.3 ± 0.9
									2,5-Dimethyl hexane	-222.5 ± 0.9
					2,3-dimethyl Butane	-177.7 ± 0.9	2,4-dimethyl Pentane	-201.9 ± 0.9	3,3-Dimethyl hexane	-220.0 ± 0.9
									3,4-Dimethyl hexane	-212.9 ± 0.9
							3,3-dimethyl Pentane	-201.3 ± 0.9	2-methyl-3-ethyl pentane	-211.1 ± 0.9
									3-methyl-3-ethyl pentane	-214.9 ± 0.9
5	-	-	-	-	-	-	2,2,3-trimethyl Butane	-204.7 ± 0.9	2,2,3-Trimethyl pentane	-220.0 ± 0.9
									2,2,4-Trimethyl pentane	-224.1 ± 0.9
									2,3,3-Trimethyl pentane	-216.3 ± 0.9
									2,3,4-Trimethyl pentane	-217.3 ± 0.9
6	-	-	-	-	-	-	-	-	2,2,3,3-Tetramethyl butane	-225.8 ± 0.9

Table 5. **Raw Data from Thermochemical Data of Organic Compounds**

Number of Endpoints	Number of Carbon Atoms									
	4		5		6		7		8	
	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)	Isomer	Enthalpy of Formation (kJ/mol)
2	n-Butane	-125.6 ± 0.7	n-Pentane	-146.9 ± 0.9	n-Hexane	-167.1 ± 0.8	n-Heptane	-187.7 ± 1.3	n-Octane	-208.6 ± 1.4
3	2-methyl Propane	-134.2 ± 0.7	2-methyl Butane	-153.7 ± 1.0	2-methyl Pentane	-174.8 ± 1.0	2-methyl Hexane	-194.6 ± 1.0	2-methyl heptane	-215.4 ± 1.5
							3-methyl Hexane	-191.3 ± 1.9	3-methyl heptane	-212.5 ± 1.3
					3-methyl Pentane	-172.1 ± 1.0	3-ethyl Pentane	-189.6 ± 1.2	4-methyl heptane	-212.0 ± 1.3
									3-Ethyl hexane	-210.7 ± 1.3
4	-	-	Neopentane	-168.1 ± 1.0	2,2-dimethyl Butane	-186.1 ± 1.0	2,2-dimethyl Pentane	-205.9 ± 1.5	2,2-Dimethyl hexane	-224.6 ± 1.3
									2,3-Dimethyl hexane	-213.8 ± 1.6
							2,3-dimethyl Pentane	-198.9 ± 1.5	2,4-Dimethyl hexane	-219.2 ± 1.3
									2,5-Dimethyl hexane	-222.5 ± 1.6
					2,3-dimethyl Butane	-178.3 ± 1.0	2,4-dimethyl Pentane	-201.7 ± 1.1	3,3-Dimethyl hexane	-220.0 ± 1.3
									3,4-Dimethyl hexane	-212.8 ± 1.6
							3,3-dimethyl Pentane	-201.2 ± 1.1	2-methyl-3-ethyl pentane	-211.0 ± 1.4
									3-methyl-3-ethyl pentane	-214.8 ± 1.4
5	-	-	-	-	-	-	2,2,3-trimethyl Butane	-204.5 ± 1.3	2,2,3-Trimethyl pentane	-220.0 ± 1.6
									2,2,4-Trimethyl pentane	-224.0 ± 1.5
									2,3,3-Trimethyl pentane	-216.3 ± 1.5
									2,3,4-Trimethyl pentane	-217.3 ± 1.8
6	-	-	-	-	-	-	-	-	2,2,3,3-Tetramethyl butane	-225.6 ± 1.4