

Using an Internet-based Chemical Database

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1 Aim

The aim is to use the database provided by The National Institute of Standards and Technology (NIST), founded in 1901.

2 Introduction

To use a database we need to ensure this database is authentic, which for this database can be recognized by its `.gov` domain TLD, which indicates it is a governmental organization and have been verified for identity. Except that, online databases with domain ending with `.edu` also indicates an verified educational institution which oftenly is also authentic. But for this particular lab, the source `nist.gov` is preferable because of the speciality of the lab requirement - using a chemical **database**.

3 Materials

No materials are needed.

4 Apparatus

1. Laptop or equivalent technology
2. Access (internet or intranet) to the database
3. Office Excel or equivalent software

5 Safety Measures

Safety measures on the usage of internet and technology is emitted due to the limit on such description will contribute valuable information to this lab report.

6 Procedure

1. Navigate to <https://webbook.nist.gov/chemistry/> using an internet browser
2. Click *Formula* under *General Searches*
3. Enter the chemical formula in the corresponding field and click *Search*
4. Choose the right one in all the species matching the search result
5. Click *Gas phase thermochemistry data*
6. Find the $\Delta_c H^\theta$ data
7. Record the corresponding data to the table
8. Graph data as Number of carbon atoms vs. Heat of combustion

7 Data Collection

Choosing from Multiple Data

- If there's multiple data corresponding to one chemical substance, the **latest published data** will be used because it:
 - oftenly provides more accurate result due to the usage of optimized equipments;
 - oftenly provides more advanced and scientific ways to calculate such data;
 - oftenly have more numbers of being referenced than the old ones, creating a higher probability that an error will be found.

# of C atoms	Name	Formula	$\Delta_c H^\theta$ (kJ mol ⁻¹)	Uncertainty (kJ mol ⁻¹)	Molecular Mass (g mol ⁻¹)
1	Methane	CH ₄	-890.7	0.4	16.0425
2	Ethane	C ₂ H ₆	-1411.2	0.3	30.069
3	Propane	C ₃ H ₈	-2057.8	1.1	44.0956
4	Butane	C ₄ H ₁₀	-2877.5	0.63	58.1222
5	Pentane	C ₅ H ₁₂	-3535.4	0.96	72.1488
6	Hexane	C ₆ H ₁₄	-4163	20	86.1754
7	Heptane	C ₇ H ₁₆	-4817	0.8	100.2019
8	Octane	C ₈ H ₁₈	-5430	0.1	114.2285

Table 1: Data [1]

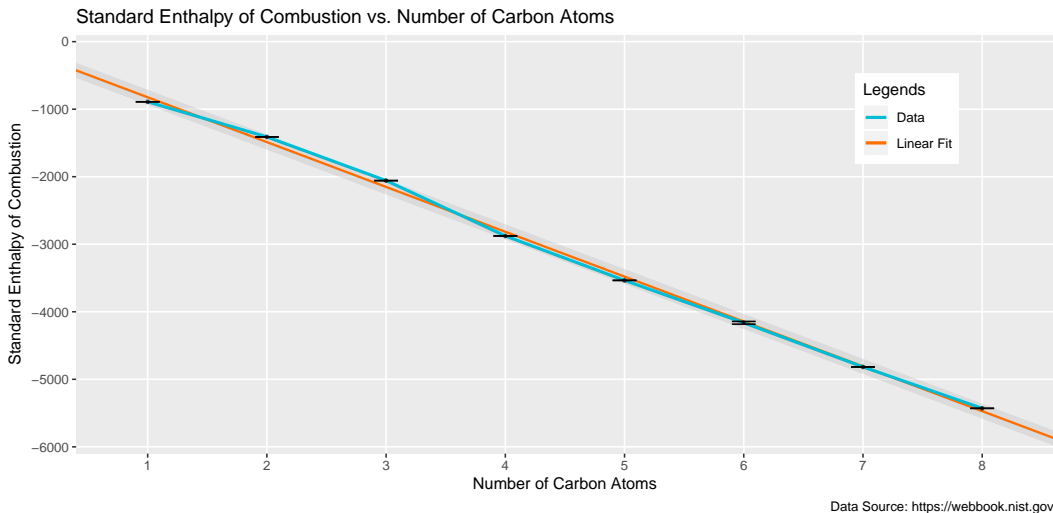


Figure 1: $\Delta_c H^\theta$ vs. # of C atom
 Linear Fit Equation: $y = -664.02x - 159.74$

8 Analysis

The combustion reaction equation for CH_4 is:
 Methane



From the graph we can observe a clear negative linear correlation between the number of carbon atoms and the standard enthalpy of combustion. But notice that a negative value of the standard enthalpy of combustion of a molecule indicates the enthalpy goes less than before, so we can then conclude that more the number of carbon atoms, more the enthalpy lost will there be.

This is because that when the combustion reaction happens, the covalent bond between C—H will break, causing enthalpy goes down, which indicates that this reaction is an endothermic reaction.

9 Conclusion

We can conclude that there's a negative linear correlation between the number of carbon atoms and the standard enthalpy of combustion, which indicates that it is an endothermic reaction.

References

- [1] Linstrom, Peter. NIST Chemistry WebBook, NIST Standard Reference Database 69. National Institute of Standards and Technology, 1997, doi:10.18434/T4D303.