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Laboratory Experiment

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Rocket Scientist for a Day: Investigating Alternatives for Chemical Propulsion

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Supporting Information

ABSTRACT: This laboratory experiment introduces rocket science from a chemistry perspective. The focus is set on chemical propulsion, including its environmental impact and future development. By combining lecture-based teaching with practical, theoretical, and computational exercises, the students get to evaluate different propellant alternatives. To complete the task, they need to use several important curricular concepts, such as the breaking and formation of bonds, redox reactions, and thermodynamics. They also apply basic computational electronic structure calculations to investigate the energetic content of hitherto nonexisting alternatives. Finally, actual chemical rocket propulsion is demonstrated through the assembly and testing of a model rocket motor, employing a commercially available kit. The full experiment was developed for upper-level high school classes and is completed in a 3-h lab period. The experiment, or parts of it, has also been successfully used both in undergraduate programs and continuing education for teachers.

KEYWORDS: *High School/Introductory Chemistry, First-Year Undergraduate/General, Physical Chemistry, Interdisciplinary/Multidisciplinary, Hands-On Learning/Manipulatives, Applications of Chemistry, Calorimetry/Thermochemistry, Computational Chemistry, Covalent Bonding, Oxidation/Reduction*

In 1919, Robert H. Goddard, the father of modern rocketry, published the pioneering *A Method of Reaching Extreme Altitudes*.[1] Seven years later, in 1926, he launched the world's first liquid rocket, which was propelled by gasoline and liquid oxygen. Since then, the development of rocket propulsion and the exploration of space have progressed at a great rate. Continuous exploration of space is necessary for several reasons, such as advancing of our understanding of the solar system and even ensuring the long-term survival of our species.[2−4] Even though future interplanetary missions are likely to be propelled by high-power plasma rockets[5] and ion engines,[6] launch vehicles and navigational thrusters will rely on chemical propulsion for the foreseeable future.

The majority of current space launchers are powered by solid rocket propellants in one or several of their stages. The main components of such solid propellants are the oxidant, typically ammonium perchlorate (AP, $NH_4^+ClO_4^-$), the fuel, which is commonly aluminum (Al), and a polymer matrix, typically hydroxyl terminated polybutadiene (HTPB). Such a propellant displays excellent performance characteristics; however, its combustion results in various environmentally hazardous exhaust products. For example, the recently decommissioned American space shuttles consumed 998 tons of AP-based propellant,[7] forming the equivalent of 578 tons of concentrated hydrochloric acid during launch (Figure 1).[8] Such exhaust acidifies groundwater and affects local ecosystems as well as the overall environment. The main energy-producing step can be summarized by the following redox reaction:

Figure 1. The Launch of space shuttle Atlantis.[9].

$$6NH_4ClO_4(s) + 10Al(s) \rightarrow 5Al_2O_3(s) + 6HCl(g) + 3N_2(g) + 9H_2O(g)$$

To enable more sustainable ways to explore space, the development of new oxidants and fuels are necessary.

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Ammonium dinitramide (ADN, $NH_4^+N(NO_2)_2^-$)[10] is an example of a chlorine free, and more environmentally benign oxidant that is being considered as a possible AP-replacement.[8,10−,13] Unfortunately, several problems regarding stability and chemical compatibility complicates the development and implementation of such new propellants.[12,14] To solve these problems, and to find new alternatives, tools such as quantum chemical calculations are becoming increasingly important.[8,14,15]

In this laboratory experiment, students are introduced to the exciting chemistry of rocket science. Using the well-known American space shuttles as models,[16,17] different propulsion systems are covered in lecture form, and a discussion is held on how chemical reactions can result in such massive release of energy. The students work with redox reactions and enthalpy calculations to determine the energy content of different propellants. They also learn how to apply a quantum chemistry program to theoretically investigate the energy content of hitherto nonexisting molecules with possible propellant potential. Finally, a joint construction and testing of a commercially available model rocket motor is performed.

■ THE EXPERIMENT

The experiment is divided into several parts, all connected through a lecture covering rocket science in general and chemical applications in particular. Further details on the different parts can be found in the Supporting Information. Initially, the students watch footage from a space shuttle launch.[18] From there, the discussion goes into what a propellant actually is, what types and amounts that were used during shuttle launch and the resulting environmental impact. The focus is mainly on the solid rocket propellant as it is the most troublesome component from an environmental perspective. The main combustion reaction of a propellant is shown, thereby going into redox processes. At this point, a method of balancing redox reactions is also described briefly.

After this part, the students are allowed to start assembling the model rocket motor, which is, in principle, very much similar to a space shuttle SRB (solid rocket booster, Figure 2).

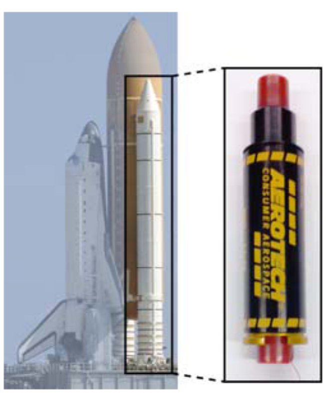

Figure 2. A space shuttle SRB and a model rocket motor.[9]

This is done in groups, of sizes depending on the number of available motor kits. After all groups finish, one motor is selected for the demonstrative launch that is performed at the end of the lab period.

Next, the principle of how a rocket actually creates thrust is discussed. Energetics of bond breaking and bond forming are also covered, and enthalpies of reaction ($\Delta H_r°$) are introduced. Concepts, such as activation energies and exo- and endothermic reactions are mentioned briefly. This is followed by chemical calculation exercises. The students are allowed to use tables of bond energies and enthalpies of formation ($\Delta H_f°$) to solve a number of problems (balancing redox equations is required in this part). Most importantly, the energetic contents of different propellants are calculated, showing the energetic superiority of the H_2/O_2 system (the problem being its low density). The calculations also show the potential of the promising ADN oxidizer.

Following a 15-min break, the lecture continues and ADN is introduced as an environmentally friendly replacement for AP. Its history and chemistry are described briefly together with some of its problems, which include unpredictable behavior in the solid state and incompatibility with commonly used polymer matrices. At this point, computational modeling through quantum chemical calculations is introduced as an important tool for understanding these processes, as well as a way to theoretically investigate the potential of new, presently nonexisting, molecules. A short introduction to quantum chemistry is given, and the Schrödinger equation is presented. Basic differences between the computational methods that will be used are also explained and a few theoretical, currently nonexisting, propellant candidates are shown. Out of those, tetrahedral N_4 is chosen as the subject for computational investigation. Tetrahedral N_4 has been the focus of considerable research efforts in recent years.[19,24,25] This is motivated by its high-energy content, spectacular nature, and possible applicability in futuristic chemical propulsion engines. Its decomposition (to molecular nitrogen, N_2) is also environmentally friendly. However, the choice of N_4 in this lab is primarily made because of the simplicity of its geometry, which simplifies the computational exercise compared to more complicated molecular systems, such as ADN.

After reading a quick instruction on how the computer program (Hyperchem, a versatile molecular modeling environment[20−23]) works, the students start by drawing and optimizing the structure of molecular nitrogen using a semiempirical model (PM3). Density functional theory (DFT) is then used to calculate its total energy. When applying the same strategy on the hypothetical compound N_4, it is shown that the tetrahedral structure is a theoretically stable conformation.[24,25] Having calculated its total energy, the students can also estimate the energy that is released when N_4 breaks apart into two N_2, thereby showing its theoretical potential as a rocket propellant candidate. The computational part of the exercise can easily be modified to accommodate the use of program packages other than Hyperchem.

The session is concluded with a short summary, after which the students and the instructor go outside and launch the model rocket using one of the assembled motors (Figure 3). Because of the large space required to launch the rocket, a model was built to enable motor testing without actual rocket launch (see Supporting Information).

■ HAZARDS

Model rocket motors are categorized as toy propellant devices (hazard class 1.4S). Carefully consult the supplied assembly description before using the product. MSDS files for the products are available at the manufacturer's Web site.[26]

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Figure 3. Astronaut Christer Fuglesang with our model rocket.

DISCUSSION

The experiment is currently included among our school programs and has been tested on several upper-level high school classes in our laboratory facilities at the House of Science (Vetenskapens Hus), in Stockholm, Sweden.[27] Generally, a 3-h lab period is required for the experiment. Different parts of the experiment have also been used in other settings, including pure lecture form and as molecular modeling computer exercises, for students and teachers of various age groups.

Our experiences have shown that students generally are highly interested in this subject and that it provides a good way to increase the motivation for some of the more theoretical parts of the curriculum, such as stoichiometry, redox chemistry, and enthalpy calculations. The structure of the lab, that is, alternating lecturing with group and more individual-based exercises, also helps the students to maintain their concentration throughout the lab. In some cases, however, depending on the students' prior knowledge, more assistance from the instructor was needed for the students to complete the more complicated calculation exercises. The computational modeling exercise adds an authentic and current feel to the experiment. Many students are curious of computational chemistry and this is a good way to introduce the concept and provide inspiration. The model rocket motor construction part, although a minor part of the experiment, adds value due to its purely practical character. Group sizes of 2−3 students work best, but larger groups are also feasible. This part also makes for a great finish, when the group that correctly assembles the motor in the shortest time gets to launch it together with the instructor and the rest of the class.

CONCLUSIONS

This laboratory experiment introduces rocket science from a chemistry perspective, focusing on rocket propellants and their environmental impact. By combining lecture-based teaching with practical, theoretical, and computational exercises, the students get to work with several important curricular concepts including bond breaking and bond forming, redox chemistry, and thermodynamic enthalpy calculations. They also gain insight into the basics of how rocket propulsion works, as well as current research in chemical rocket science. Although the laboratory experiment has mostly been tested with upper-level high school students, the experiment, or parts of it, has also proved to be interesting for several other age groups.

ASSOCIATED CONTENT

Supporting Information

Table with equipment; detailed procedures with comments and pictures; answers to the exercises; student handout; PowerPoint presentation; movie clips. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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(27) House of Science (Vetenskapens Hus) is a Swedish academic education center that aims to bring about greater interests in science

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subjects and allow the young to try science for real. It was initiated in 2001 as a collaboration between KTH (Royal Institute of Technology) and Stockholm University. http://www.vetenskapenshus.se/ (accessed Jun 2012).

Supporting Information

Rocket Scientist for a Day:

Investigating Alternatives for Chemical Propulsion

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Table of Contents

Supplies and Materials

Product Name	Vendor	Model No.	Price	Safety	Picture
Model rocket motor construction					
RMS-24/40 Motor	Aerotech[1]	91241	$39.99	MSDS[2]	Picture 1
D9-7W (reload kit, 3-pak)	Aerotech[1]	40907VR	$18.99	MSDS[2]	Picture 2
Model rocket and launch (optional)					
Interlock Controller	Aerotech[1]	89381	$73.99	-	Picture 3
Mantis Launch Pad	Aerotech[1]	89281	$116.99	-	Picture 4
Arreaux Rocket Kit	Aerotech[1]	89013	$59.99	-	Picture 5
12V Car Battery	-	-	-	-	-
Model rocket special launch (optional)					
Special Launch Pad	Author-made	Homemade device. Use at own risk			Picture 6
Computational calculations[3]					
HyperChem™ Professional Release 8.0.7 for Windows					
Student version: $89; Full version: $995 (academic), $1495(commercial)					
Contact Hypercube Inc. for question about trial versions etc.					

Lab Description with Presentation Comments

Slide 1: Starting slide

Slide 2: The outline of the experiment is presented for the students.

Slide 3: Movie clip of a space shuttle launch is shown. Comments are made on the enormous cloud of smoke that is formed. The students discuss what it could consist of (water, carbon dioxide, byproducts etc.).

Slide 4: The environmental aspect of space shuttle launch is discussed.

Slide 5: Explaining important differences between a fuel, an oxidizer and a propellant.

Slide 6: The different parts of a space shuttle are explained.

Slide 7: Discussion about how heavy a fully loaded space shuttle actually is (comparison with a large airplane). The picture shows how large part of the weight that consist of propellant.

Slide 8: The launch procedure is described in detail.

Slide 9: The different engines are described.

Slide 10: The different propellant systems are presented and their pros and cons are discussed.

Slide 11: Focus is set on the SRB and the combustion reaction (redox) is shown in detail. Notice the formation of hydrochloric acid.

Slide 12: One strategy to balance redox reactions is described briefly.

Slide 13: The SRB is compared to a commercial model rocket motor.

Slide 14: A movie clip of a rocket launch, employing a model rocket motor, is shown. The students are now given kits for assembly of a model rocket motor. This exercise is performed in groups.

Slide 15: How the rocket creates thrust through the formation of gases is described. Connections are made to Newton's third law of motion.

Slide 16: Getting into how all this energy can be released from just igniting a few chemical compounds (bond breaking and bond forming).

Slide 17: Calculations of reaction energies using bond energies are exemplified.

Slide 18: Connections are made to important concepts such as, activation energy, transition states and exo-/endothermic reactions.

Slide 19: Enthalpies of formation are introduced as a more exact way to estimate reaction energies.

Slide 20: The students get to solve the calculation exercises provided in the student handout.

A 15 minute break is allowed at this point.

Slide 21: ADN is presented as a possible alternative to AP.

Slide 22: Some applications and current limitations of ADN are discussed. Quantum mechanical calculations are mentioned as a method to increase the understanding of ADN's chemistry.

Slide 23: Background on quantum chemical calculations.

Slide 24: Short introduction to quantum mechanics/quantum chemistry.

Slide 25: The Schrödinger equation and its different parts are described.

Slide 26: The quantum chemical models that are used are described briefly.

Slide 27: Three possible propellant candidates are presented. Two of them have been detected experimentally, but not yet N_4. Is it an energetically plausible structure?

Slide 28: The students perform computer aided quantum mechanical calculations from the student handout.

Slide 29: The experiment is summarized.

Slide 30: A movie clip of the model rocket launch is shown.

After this, one of the built model rocket motors are used to launch a rocket (or demonstrated by the "reverse launch" (see below)).

Model Rocket Motor Construction[4]

Description is provided in the student handout.

Note to the instructor

For initial assembly, please consult the complete assembly description of the model rocket motor product currently available on the market. It is included with the item when purchased.

The description below has been modified by the authors due to the fact that a few steps were made by the instructor prior to the experiment. Examples include greasing of the O-rings and assembly of the delay element. This was done to make the process easier and better adapted to an event where motors need to be assembled and disassembled several times before actually being used.

For safety reasons, the igniter was also inserted by the instructor just prior to use of the model rocket motor. The ejection charge was also removed because the motors were, in the majority of cases, tested on the ground (*see above*) and not used to launch an actual rocket.

Chemical Calculation Exercises with Answers[5]

1) Estimate the enthalpy of formation ($\Delta \boldsymbol{H}_f^{\mathbf{0}}$) of water by using the table of bond energies.

$$2\ H_2 + O_2 \longrightarrow 2\ H_2O$$

To build two mole water, we first need to break two H-H bonds and one O=O bond.

$$This\ consumes: \left((2 \times 432\ kJ/mol\ ) + 495\ kJ/mol\right) = 1359\ kJ/mol$$

And we form four O-H bonds.

$$This\ releases: 4 \times 467\ kJ/mol = 1868\ kJ/mol$$

The enthalpy of formation ($\Delta \boldsymbol{H}_f^{\mathbf{0}}$) corresponds to the formation of one mole water.

$$\Delta \boldsymbol{H}_f^{\mathbf{0}} = \left(0.5 \times (1359\ kJ/mol - 1868\ kJ/mol)\right) = -254.5 \frac{kJ}{mol}\ H_2O$$

(The correct value is -286 kJ/mol)

2) Ammonium dinitramide (ADN, $NH_4N(NO_2)_2$) is one of the new, more environmentally friendly, oxidants for use in rocket propellants.

a) ADN reacts with aluminum under the formation of aluminum oxide, nitrogen and water. Write a balanced redox equation for this combustion process.

$$3\ NH_4N(NO_2)_2 + 4\ Al \longrightarrow 2\ Al_2O_3 + 6\ N_2 + 6\ H_2O$$

b) Use the table of enthalpies of formation (ΔH_f^0) to calculate the enthalpy of reaction (ΔH_r^0) for the process.

$$\Delta \boldsymbol{H}_r^{\boldsymbol{0}} = \left(\left(2 \times \left(-1676 \frac{kJ}{mol}\right)\right) + \left(6 \times 0 \frac{kJ}{mol}\right) + \left(6 \times \left(-286 \frac{kJ}{mol}\right)\right)\right)$$

$$- \left(\left(4 \times \left(0 \frac{kJ}{mol}\right)\right) + \left(3 \times -148 \frac{kJ}{mol}\right)\right) = -4624\ kJ/mol$$

c) Estimate the energy that is released per gram propellant, *i.e.* a mixture of oxidant (ADN) and fuel (Al) in the right proportions.

$$Per\ gram: \left(-4624\ kJ/mol \div \left(\left(4 \times 27.0 \frac{g}{mol}\right) + \left(3 \times 124.0 \frac{g}{mol}\right)\right)\right) = \boldsymbol{-9.6\ kJ/g\ propellant}$$

3) Calculate the enthalpy of reaction, and the amount of energy that is released per gram propellant, for the following reactions.

a) The reaction between ammonium perchlorate and aluminum (main reaction in the SRBs).

$$6\ NH_4ClO_4 + 10\ Al \longrightarrow 5\ Al_2O_3 + 6\ HCl + 3\ N_2 + 9\ H_2O$$

$$\Delta \boldsymbol{H}_r^{\boldsymbol{0}} = \left(\left(\left(5 \times \left(-1676 \frac{kJ}{mol}\right)\right) + \left(6 \times \left(-92 \frac{kJ}{mol}\right)\right) + \left(3 \times 0 \frac{kJ}{mol}\right) + \left(9 \times \left(-286 \frac{kJ}{mol}\right)\right)\right)\right)$$

$$- \left(\left(6 \times \left(-296 \frac{kJ}{mol}\right)\right) + \left(10 \times 0 \frac{kJ}{mol}\right)\right)\Bigg) = -9730\ kJ/mol$$

$$Per\ gram: \left(-9730\ kJ/mol \div \left(\left(6 \times 117.5 \frac{g}{mol}\right) + \left(10 \times 27.0 \frac{g}{mol}\right)\right)\right)$$

$$= \boldsymbol{-10.0\ kJ/g\ propellant}$$

b) The formation of water from oxygen and hydrogen gas (main engine reaction).

$$2\ H_2 + O_2 \longrightarrow 2\ H_2O$$

$$\Delta \boldsymbol{H}_r^{\mathbf{0}} = \left(\left(2 \times \left(-286 \frac{kJ}{mol}\right)\right) - \left(2 \times 0 \frac{kJ}{mol}\right) + 0 \frac{kJ}{mol}\right) = -572\ kJ/mol$$

$$Per\ gram\colon \left(-572\ kJ/mol \div \left(2 \times 18.0 \frac{g}{mol}\right)\right) = \boldsymbol{-15.9\ kJ/g\ propellant}$$

c) The combustion of methyl hydrazine with nitrogen tetroxide (runs the OMS engine)

$$4\ CH_6N_2 + 5\ N_2O_4 \longrightarrow 9\ N_2 + 4\ CO_2 + 12H_2O$$

$$\Delta \boldsymbol{H}_r^{\mathbf{0}} = \left(\left(\left(9 \times 0 \frac{kJ}{mol}\right) + \left(4 \times \left(-394 \frac{kJ}{mol}\right)\right) + \left(12 \times \left(-286 \frac{kJ}{mol}\right)\right)\right)\right.$$

$$\left. - \left(\left(4 \times 54 \frac{kJ}{mol}\right) + \left(5 \times \left(-20 \frac{kJ}{mol}\right)\right)\right)\right) = -5124\ kJ/mol$$

$$Per\ gram\colon \left(-5124\ kJ/mol \div \left(\left(4 \times 46.0 \frac{g}{mol}\right) + \left(5 \times 92.0 \frac{g}{mol}\right)\right)\right) = \boldsymbol{-8.0\ kJ/g\ propellant}$$

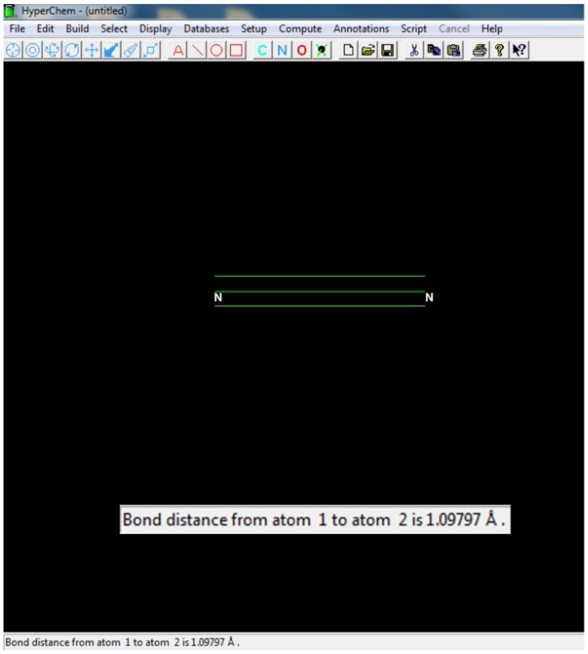
Computational Modeling Exercises with Answers

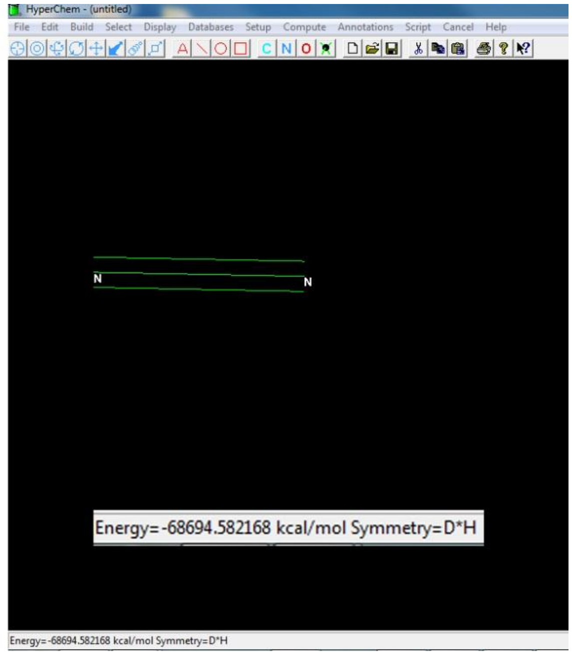
For descriptions of the actual exercises, see the student handout.

Investigate if tetrahedral N_4 is a stable molecule, and if it energetically is a candidate green rocket propellant. N_4 reacts to form two N_2.

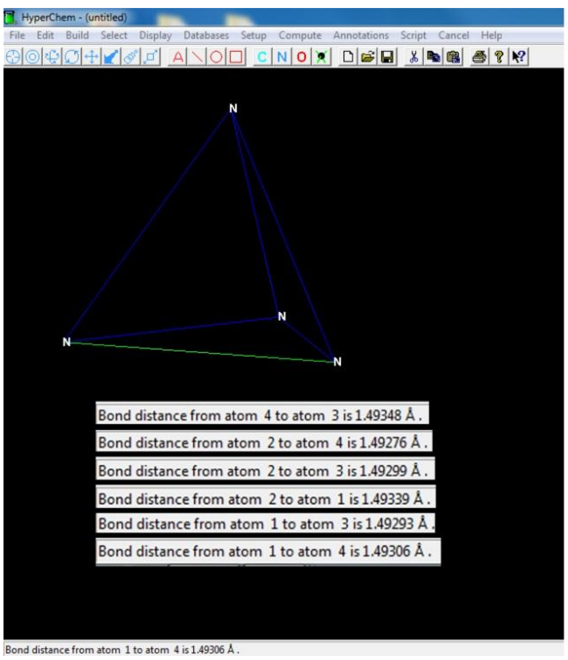
1a) Optimize the structure for the dinitrogen molecule using a semiempirical method (PM3).

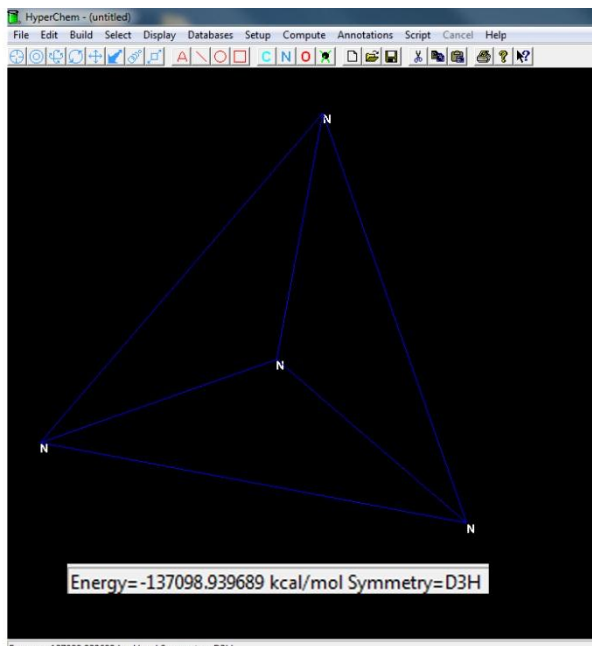
b) Employ a DFT method in order to calculate the total energy of the N_2 molecule.





2) Do the same type of calculations for tetrahedral N_4.





Screenshots are published with permission.[6]

3) Use your calculated energies to estimate the energy that is released when tetrahedral N_4 is converted to 2 N_2. Also calculate the amount of energy per gram N_4. (The calculated values are given in kcal/mol. 1 calorie (cal) = 4.184 joule (J)).

$$N_4 \longrightarrow 2\ N_2$$

$$Energy\ N_2 = -68694.6\frac{kcal}{mol} = -287418.2\ \frac{kJ}{mol}$$

$$Energy\ N_4 = -137215.4\frac{kcal}{mol} = -574109.2\ \frac{kJ}{mol}$$

$$Released\ energy = 2 \times (-287418.2\frac{kJ}{mol}) - (-574109.2) = -727\ kJ/mol$$

$$Per\ gram: \left(-727\ kJ/mol \div \left(4 \times 14.0\frac{g}{mol}\right)\right) = \boldsymbol{-13.0\ kJ/g\ propellant}$$

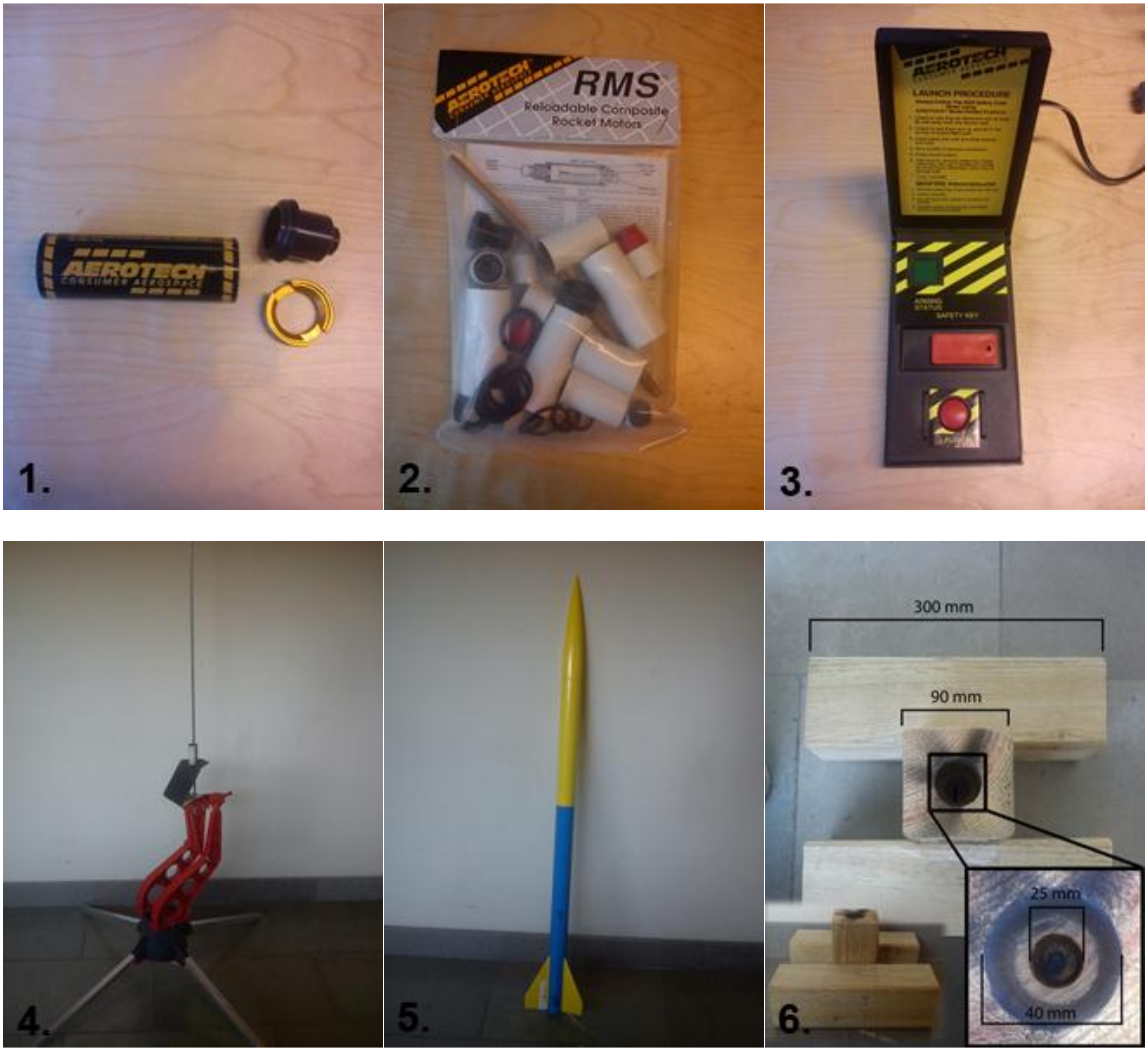
Model Rocket Launch

How to launch the model rocket is described in the instructions that come with the merchandise. In our "reversed launch", the loaded motor (upside down, without the ejection charge) was placed in the bottom of the home-built launch pad. The launch was then made according to regular procedure. More details on the measurements of the launch pad can be found in the picture section.

Student Handout

A student handout is available at the end of this document. Values for bond energies[7] and enthalpies of formations[8,9] were taken from the respective citations.

Pictures[10]


1.
AEROTECH
CONSUMER AEROSPACE
2.
AEROTECH
RMS
Reloadable Composite
Rocket Motors
3.
AEROTECH
LAUNCH PROCEDURE
SAFETY KEY
4.
5.
6.
300 mm
90 mm
25 mm
40 mm

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10. Pictures of Aerotech merchandise, displaying their logotype, are used with permission.
11. Rahm, M.; Brinck, T. *Chem. Eur. J.* **2010**, *16*, 6590-6600.
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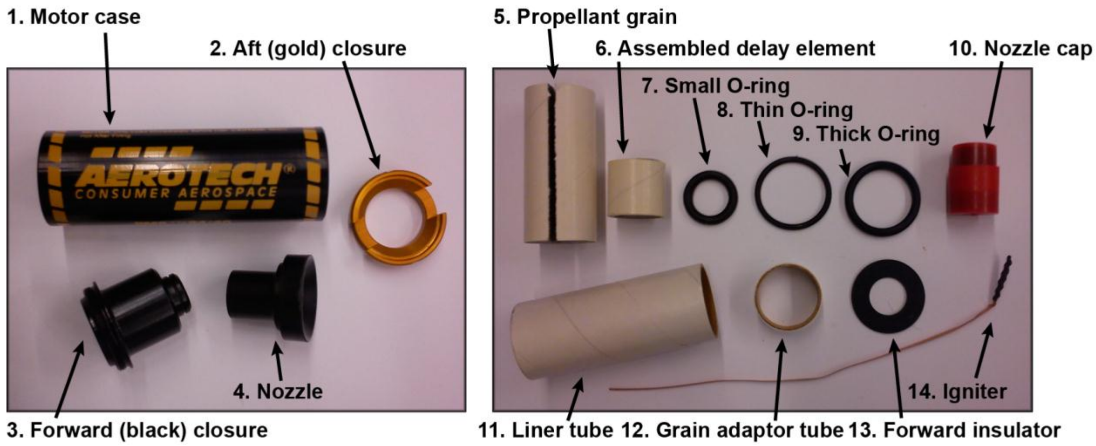
Rocket Scientist for a day

Investigating Alternatives for Environmental Propulsion

Bond-dissociation energy, BDE (kJ/mol)	
C-C	347
C-H	413
H-H	432
O-H	467
O=O	495
C=O	745
N-H	391
N≡N	941

Standard enthalpy of formation, ΔH_f^0 (kJ/mol)	
Aluminium, Al(s)	0
Aluminium oxide, Al_2O_3(s)	-1676
Ammonium dinitramide (ADN), $NH_4N(NO_2)_2$(s)	-148
Ammonium perchlorate, NH_4ClO_4(s)	-296
Carbon dioxide, CO_2(g)	-394
Nitrogen, N_2(g)	0
Dinitrogen tetroxide, N_2O_4(l)	-20
Methyl hydrazine, CH_6N_2(l)	54
Hydrochloric acid, HCl(g)	-92
Oxygen, O_2(g)	0
Water, H_2O(l)	-286
Hydrogen, H_2(g)	0

Assembly of model rocket motor



Description

- Place the small O-ring (7) in the cavity inside the forward closure (3).
- Insert the assembled delay element (6) in the forward closure (3) until it is seated against the O-ring (7). The side with a small space should be directed outwards.
- Insert the grain adaptor tube (12) in the liner tube (11) until flush with one end of the liner tube (you might need to sandpaper the inside carefully for it to fit).
- Attach a small piece of masking tape to the end of the propellant grain (5) so it covers the slot.
- Insert the propellant grain (5), taped end first, into the liner tube (11) until it is seated against the grain adaptor tube (12).

[It is important that the following steps are made with the motor held in vertical position.]

- Insert the liner assembly (5+11+12) in the motor case (1).
- Place the forward insulator (13) against the liner assembly (11) in the end where the grain adaptor tube (12) is placed.
- Place the thin O-ring (8) against the forward insulator (13).
- Gently thread the forward closure (3) into the same end of the motor case (1).

[Normally the igniter is inserted here. This will be done by the instructor at a later stage.]

- Place the nozzle (4) at the back end of the motor case (1).
- Place the thick O-ring (9) into the groove between the nozzle (4) and case (1).
- Thread the aft closure into the motor by hand. Both closures should be tightened after the igniter has been inserted by the instructor.
- Make a mall vent hole (1/16’’) in the nozzle cap (10) and place it over the nozzle (4).

Calculations

1) Estimate the enthalpy of formation (ΔH_f^0) of water by using the table of bond energies.

2) Ammonium dinitramide (ADN, $NH_4N(NO_2)_2$) is one of the new, more environmentally friendly, oxidants for use in rocket propellants.

a) ADN reacts with aluminum and form aluminum oxide (Al_2O_3), nitrogen and water. Write a balanced redox equation for this combustion process.

b) Use the table of enthalpies of formation (ΔH_f^0) to calculate the enthalpy of reaction (ΔH_r^0) for the process.

c) Estimate the energy that is released per gram propellant, *i.e.* a mixture of fuel (Al) and oxidant (ADN) in the right proportions.

3) Calculate the enthalpy of reaction, and the amount of energy that is released per gram propellant, for the following reactions.

a) The reaction between ammonium perchlorate and aluminum (main reaction in the SRBs).

$$6\ NH_4ClO_4 + 10\ Al \longrightarrow 5\ Al_2O_3 + 6\ HCl + 3\ N_2 + 9\ H_2O$$

b) The formation of water from oxygen and hydrogen gas (main engine reaction).

$$2\ H_2 + O_2 \longrightarrow 2\ H_2O$$

c) The combustion of methyl hydrazine with nitrogen tetroxide (runs the OMS engine)

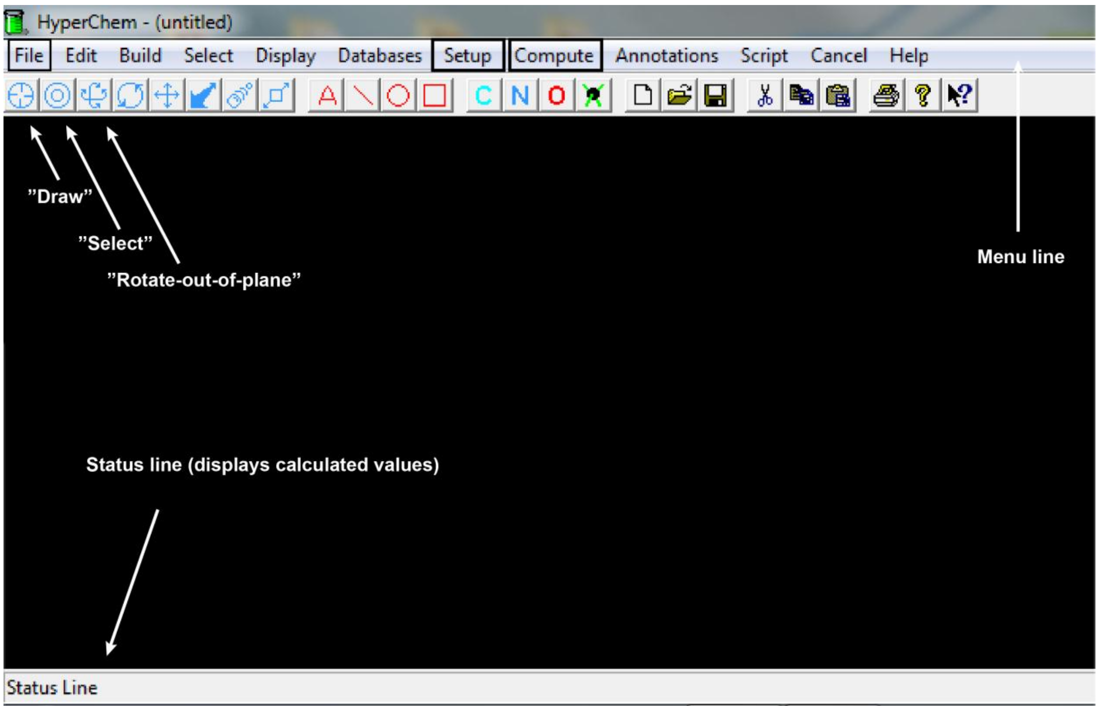
$$4\ CH_6N_2 + 5\ N_2O_4 \longrightarrow 9\ N_2 + 4\ CO_2 + 12H_2O$$

Computational modelling using HyperChem

HyperChem

HyperChem is a user-friendly program for molecular modeling (www.hyper.com).

Below is a screenshot where most of the tools and functions used in this laboratory experiment have been marked out.



Basic commands and instructions

- Double-click on the tool ”Draw” to display a periodic table where elements can be selected. This element will then be selected until a new choice is made.
- When an element has been selected, left-click on the screen to draw this element.
- To create a bond, place the mouse cursor over an element, left-click, hold and move the cursor to the another element and release.
- Right-click on an object to delete it.
- Left-click on a bond to change the bond order (create double or triple bond)
- Select something by using the ”Select”-tool and left-click. Right-click to deselect.

Modelling exercises

Investigate if tetrahedral N_4 is a stable molecule, and if it contains enough energy to function as a green rocket propellant. N_4 reacts to form 2 N_2.

a) Optimize the structure for the nitrogen molecule using a semiempirical method (PM3).

- Draw two nitrogen atoms.
- Connect the atoms with a bond to create the N_2 molecule. Remember that the nitrogen molecule is held together by a triple bond.
- Under **Setup** in the menu line, select ”Semi-empirical” and then “PM3”.
- Press **Compute** on the menu line, followed by ”Geometry optimization” (Polak-Ribiere). Click OK.
- Use the ”Select” tool and select the N_2 bond. Note the calculated bond length.

b) Use Density Functional Theory (DFT) to calculate the total energy of the N_2 molecule.

- Under **Setup**, select DFT (”Density Functional…”) and then “”Medium basis set”. Press “Exchange correlation” and select “Use combination potential” and “B3LYP”.
- Under **Compute**, press “Single Point” and note the calculated total energy.

c) Create a new working window and make the same calculations on tetrahedral N4 (see a) and b)). However, after having drawn out and connected the three first nitrogen atoms, use the “Rotate out-of-plane” tool to rotate the structure in three dimensions. Then you can draw the fourth nitrogen atom. Don’t forget to note bond lengths and total energy.

d) Use your calculated energies to estimate the energy that is released when tetrahedral N_4 is converted to two N_2. Also calculate the amount of energy per gram N_4. (The calculated values are given in kcal/mol. 1 calorie (cal) = 4.184 joule (J)).

$$N_4 \longrightarrow 2\,N_2$$

Extra assignment: Investigate the stability of other potential structures of N_4

Appendix: supporting material for calculations

Step-by-step description for balancing redox equations

- Write down the basic reaction, i.e. the compounds that react and are formed.
- Use oxidation numbers to identify which elements that have been oxidized and reduced, respectively. The sum of a compounds oxidation states are equal to its charge. Remember that elements in the ground state have the oxidation number 0 and that hydrogen normally has the oxidation state +I, and oxygen +II in chemical compounds.
- Use the information above to divide the basic reaction into two half-reactions, one oxidation (ox.) and one reduction (red.) part. Treat these half-reactions separately.
- Balance both sides with regard to all atoms except oxygen and hydrogen. Do this by multiplying the compounds with positive integers.
- Balance oxygen by adding water (H_2O) at the appropriate side of the equation.
- Balance hydrogen by using:
  - Protons (H^+) in acidic solution
  - An equal number of water (H_2O) and hydroxide (OH^-) molecules on each side in basic solution (this gives a net addition of H^+).
- Balance the charge using electrons (e^-).
- Multiply the two half-reactions by positive integers so that an equal number of electrons are released (in ox.) and taken up (in red.), respectively.
- Combine the half-reactions and simplify the combined redox equation

1) Estimate the enthalpy of reaction (ΔH_f^0) for the formation of ammonia from nitrogen and hydrogen by using the table of bond energies.

The reaction: $N_2 + 3\ H_2 \longrightarrow 2\ NH_3$

Broken bonds: 3 H-H, 1 N≡N, which consumes $(3 \times 435) + 945 = 2250\ kJ$

Bonds formed: 6 N-H, which release $6 \times 389 = 2334\ kJ$

Total: $2250 - 2334 = -84\ kJ$ is released during the reaction (in this case is $\Delta H_r^0 = 2 \times \Delta H_f^0$).

b) Use the table of enthalpies of formation (ΔH_f^0) to calculate the enthalpy of reaction (ΔH_r^0) for the combustion of octane in oxygen.

The combustion reaction: $2\ C_8H_{18} + 25\ O_2 \longrightarrow 16\ CO_2 + 18\ H_2O$

$$\Delta H_r^0 = \Delta H_{f\,(product)}^0 - \Delta H_{f\,(starting\ material)}^0$$

$$\Delta H_r^0 = \left((16 \times \Delta H_{f\,(CO_2)}^0 + 18 \times \Delta H_{f\,(H_2O)}^0) - (2 \times \Delta H_{f\,(C_8H_{18})}^0 + 25 \times \Delta H_{f\,(O_2)}^0)\right)$$

$$\Delta H_r^0 = \Big(\big(16 \times (-394)\big) + \big(18 \times (-296)\big)\Big) - \Big(\big(2 \times (-250)\big) + (25 \times 0)\Big) = -10952\ kJ$$

If you want to make the calculation per gram propellant, you have to divide it with the molar mass of the propellant in correct proportions.

$$-10952 \div \left(2 \times M_{C_8H_{18}} + 25 \times M_{O_2}\right) = -10952 \div \big((2 \times 114) + (25 \times 32)\big) = -10.6\ kJ/g$$

Rocket Scientist for a Day

Investigating Alternatives for Enviromental Propulsion

Slide show layout has been modified in order to meet copyright criteria

VETENSKAPENS HUS

Rocket Scientist for a Day

- Launching a space shuttle
- The chemistry behind launching and powering the shuttle
- Calculations and comparison of different rocket propellants
- Computer modelling as a tool for investigating new alternatives
- Construction and test of a model rocket engine

Here we showed a short part of a NASA video from the launch of space shuttle Atlantis (STS-129).

The original video was accessed via youtube:

http://www.youtube.com/watch?v=zsJpUCWfyPE

(accessed on Mar 2012)

Rocket Propellants – Environmental Issues?

- 550 tons concentrated HCl is released in the atmosphere
  - Acidification
  - Toxic compounds in ground water
  - Ozone layer depletion (through chlorine radicals)
- Highly toxic compounds power the smaller engines
  - Fueling
  - Launch

Photo: NASA

What is a Rocket Propellant?

- Combustion
  - A chemical process where a **fuel** reacts with an **oxidant** under the formation of heat.
- Propellant = fuel + oxidant
  - A material that can combust itself and produce large amounts of a gaseous products at a rapid rate.

Photo: NASA

Structure of the Space Shuttle

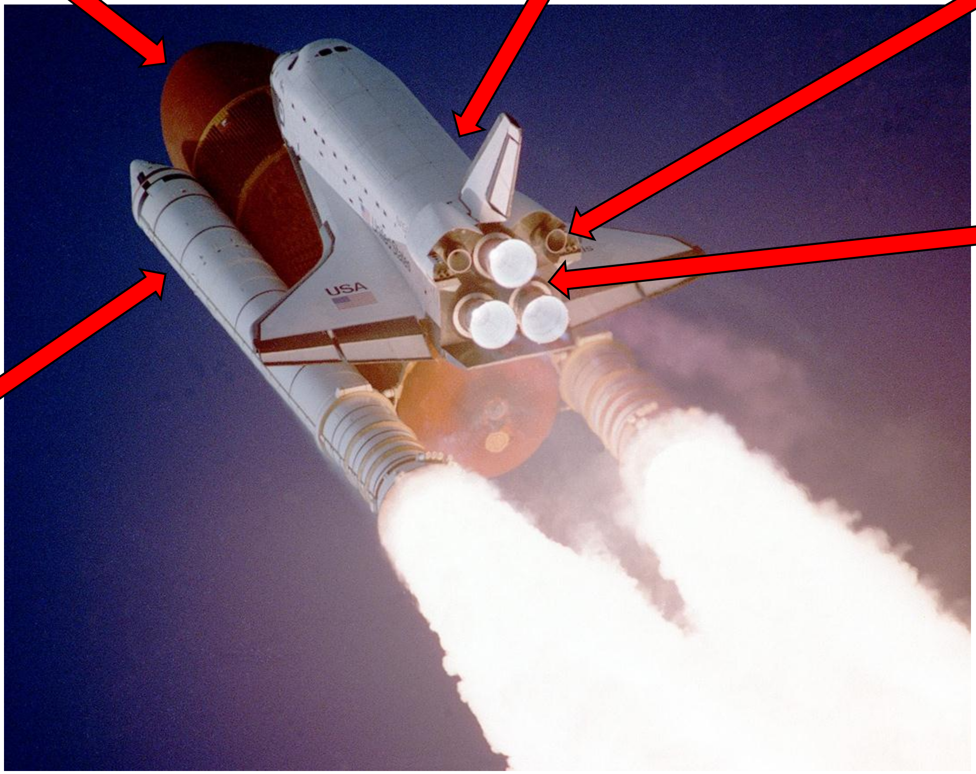
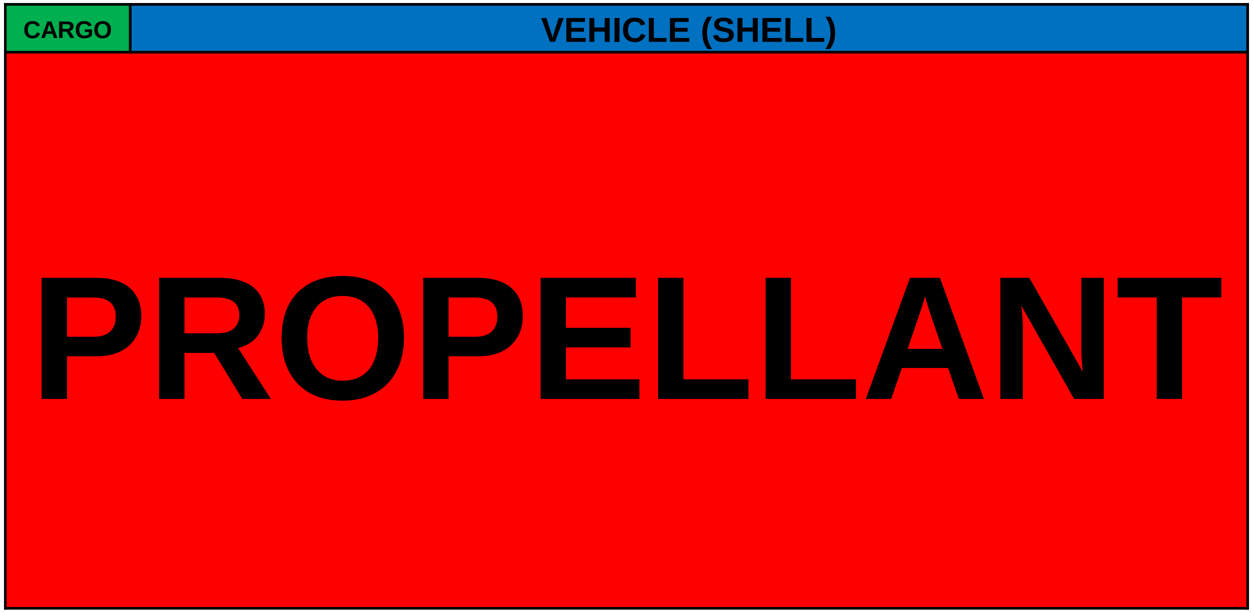


Photo: NASA

The Space Shuttle: Weight Distribution



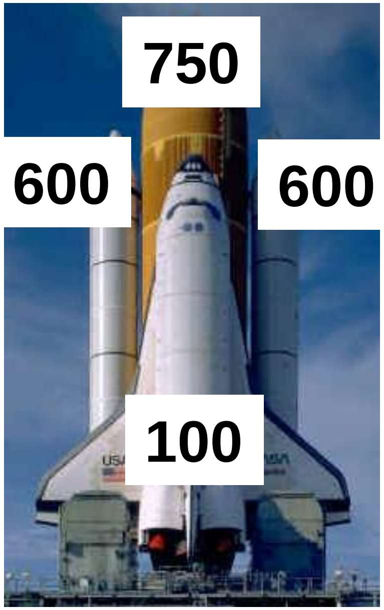


Photo: NASA

Total weight: >2000 tons

Space Shuttle Launch: Step by Step

- T minus 31 s – Computer onboard the shuttle takes over
- T minus 6.6 s – Main engine ignition
- T – SRB ignition, followed by lift-off
- T plus 2 min – SRBs separate from shuttle
- T plus 8.5 min – Main engine shut-off
- T plus 9 min – ET separates from shuttle
- T plus 10.5 min – OMS-engines places the shuttle in low orbit

Propellants in NASA Space Shuttles

OMS-engines (orbital maneuvering system)

Main engines

SRBs – solid rocket boosters

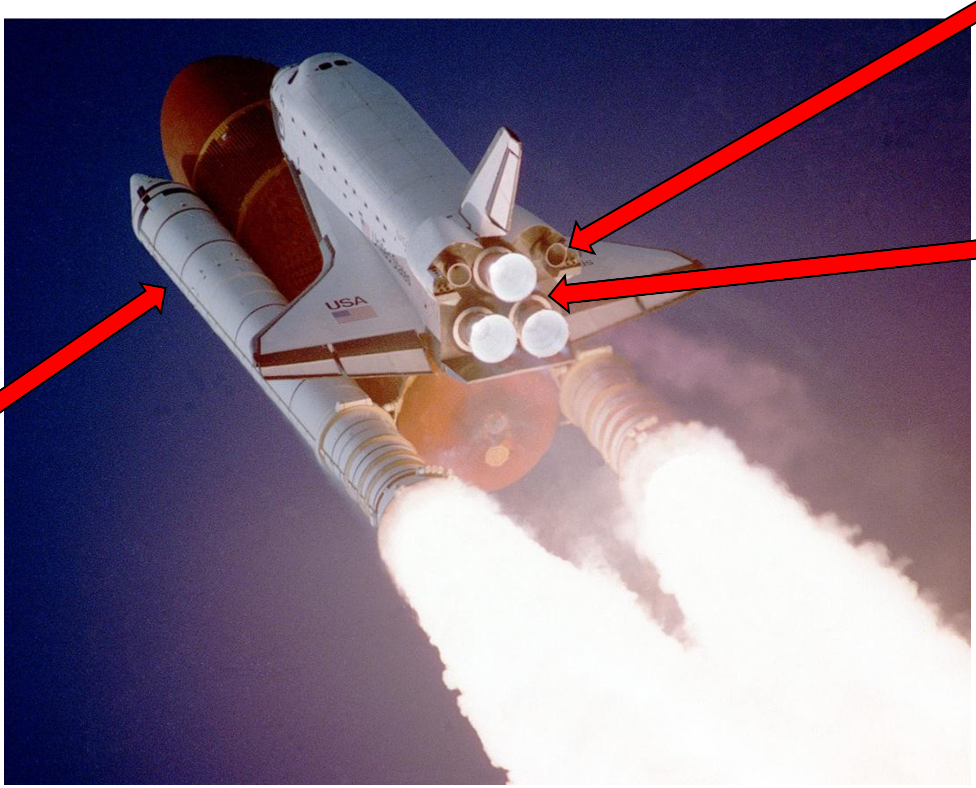


Photo: NASA

Propellants in NASA Space Shuttles

- Main engines
  - Oxidant: O_2(l)
  - Fuel: H_2(l)
  - Environmentally friendly
  - Low density

- SRBs (solid propellant)
  - Oxidant: Ammonium perchlorate, NH_4ClO_4(s)
  - Fuel: Aluminum(s) (+ plastic binder)
  - High density
  - Harmful to the environment

- OMS engines
  - Oxidant: Nitrogen tetroxide, N_2O_4(l)
  - Fuel: Methyl hydrazine, CH_6N_2(l)
  - Hypergolic
  - Toxic

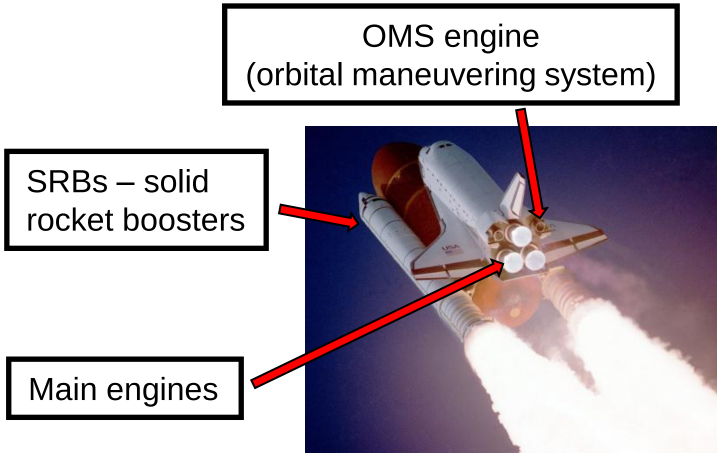
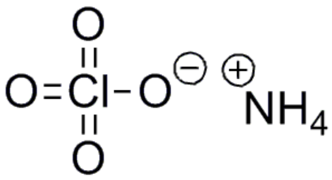


Photo: NASA

SRB – the Environmental Issue

68% Ammonium perchlorate (oxidant)



18% Aluminum (fuel)

14% Plastic binder (HTPB/isocyanate polymer)

$$6\ NH_4ClO_4 + 10\ Al \longrightarrow 5\ Al_2O_3 + 3\ N_2 + \mathbf{6\ HCl} + 9\ H_2O$$

A **redox** reaction

Balancing Redox Equations

O: - II
H: + I

$$\overset{0}{\mathrm{NH_4ClO_4 + Al}} \longrightarrow \overset{+III}{\mathrm{Al_2O_3}} + N_2 + HCl + H_2O$$

ox. $(2\,Al + 3\,H_2O \longrightarrow Al_2O_3 + 6\,H^+ + 6\,e^-) \times 5$

red. $(2\,NH_4ClO_4 + 10\,H^+ + 10\,e^- \longrightarrow N_2 + 2\,HCl + 8\,H_2O) \times 3$

$$10\,Al + 15\,H_2O + 6\,NH_4ClO_4 + 30\,H^+ + 30\,e^- \longrightarrow 5\,Al_2O_3 + 30\,H^+ + 30\,e^- + 3\,N_2 + 6\,HCl + 24\,H_2O$$

$$\boxed{10\,Al + 6\,NH_4ClO_4 \longrightarrow 5\,Al_2O_3 + 3\,N_2 + 6\,HCl + 9\,H_2O}$$

1) Balance both sides with regard to all atoms except oxygen and hydrogen
2) Balance oxygen by adding H_2O
3) Balance hydrogen with H^+ (OH^- and H_2O if alkaline solution)
4) Balance charge with e^-
5) Multiply the two half-reactions by positive integers so the electrons evens out
6) Combine the half-reactions and simplify the combined redox equation

The Structure of an SRB

Photo: NASA

Here we displayed how an SRB is constructed. The school of Aeronautics and Austronautics at Purdue university has a nice examples on their website:

https://engineering.purdue.edu/AAE/Research/Propulsion/Info/rockets/solids

(accessed on Mar 2012)

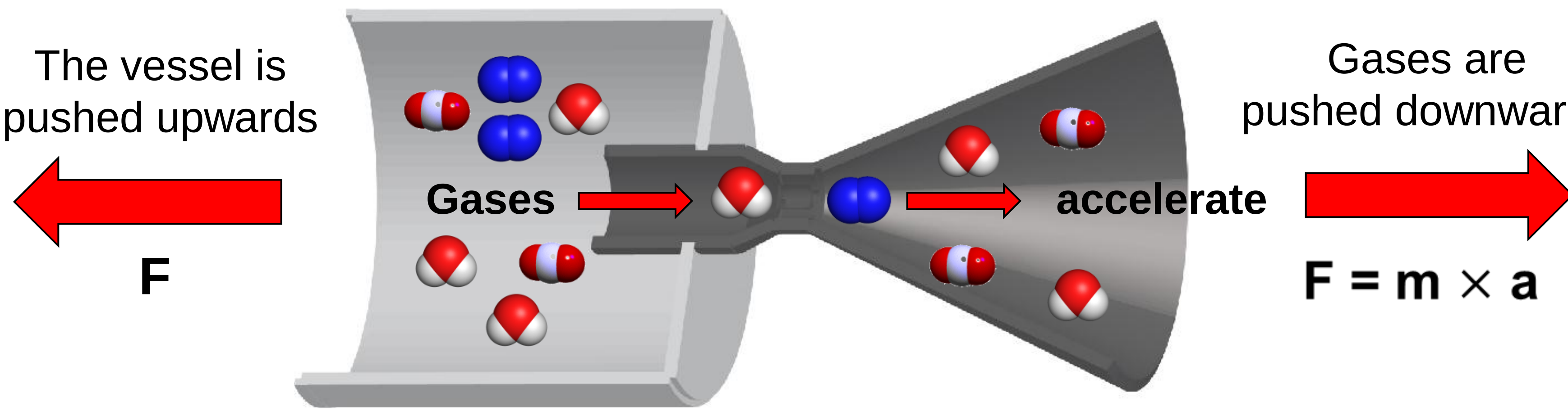
Part 1: Construction of a Model Rocket Engine

Here we show a movie of when we launch a model rocket using the model rocket engine. The movie file is provided online in the supporting information section.

Astronaut Christer Fuglesang with our model rocket

How do the Rockets Create Thrust?

$$6\ NH_4ClO_4(s) + 10\ Al(s) \longrightarrow 5\ Al_2O_3(s) + 3\ N_2\mathbf{(g)} + 6\ HCl\mathbf{(g)} + 9\ H_2O\mathbf{(g)}\ \mathbf{+\ Energy}$$



Newton's third law of motion:

"For every force there is a reaction force that is equal in size, but opposite in direction"

Where do the Energy Come From?

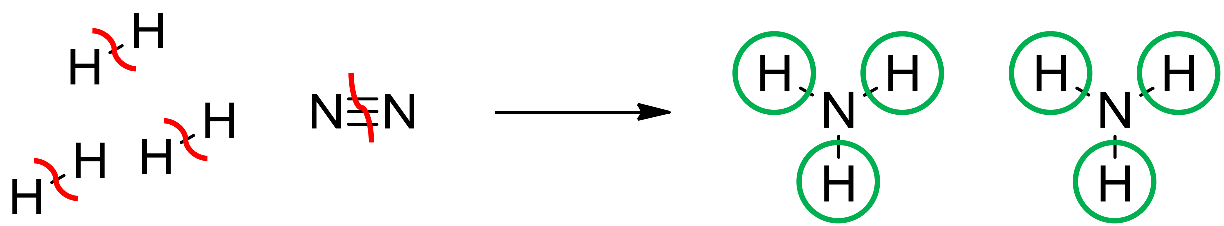
- The main changes are in the chemical bonds
- Breaking bonds requires energy, forming bonds releases energy

Bond dissociation energies (BDE):
H-H : 435 kJ/mol
C-C : 347 kJ/mol
C-H : 414 kJ/mol
O-H : 464 kJ/mol
N-H : 389 kJ/mol
O=O : 497 kJ/mol
C=O : 736 kJ/mol
N≡N : 945 kJ/mol

A Calculation Example

- Calculate the reaction energy (enthalpy of reaction, $\Delta H_{reac}{}^{0}$) for converting nitrogen and hydrogen to ammonia

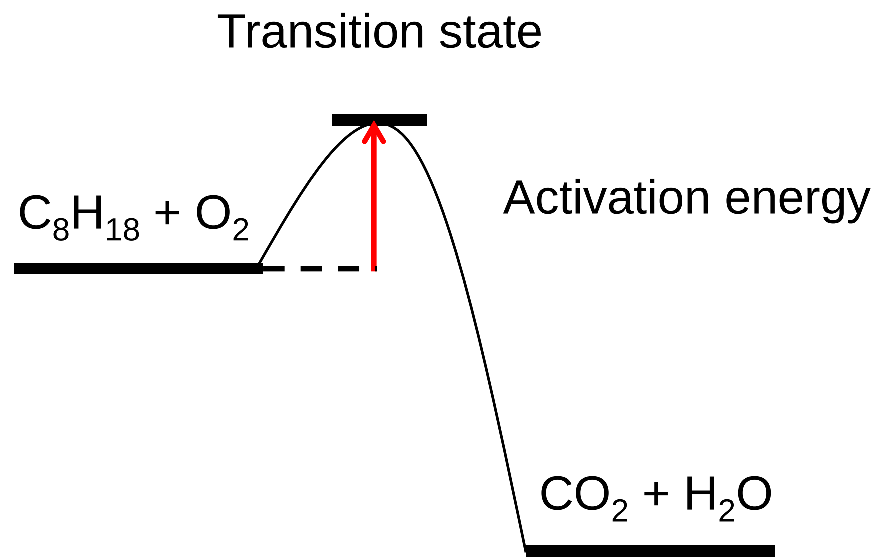
$$N_2 + 3\,H_2 \longrightarrow 2\,NH_3$$



- Broken bonds:
  - 3 H-H, 1 N≡N which require (3x436) + 941 = 2249 kJ/mol
- Formed bonds:
  - 6 N-H which releases 6x391 = 2346 kJ/mol

$\boxed{\text{Total: 2249 – 2346 = -97 kJ/mol is released during the reaction}}$

Fuel Combustion



$$\boxed{2\,C_8H_{18} + 25\,O_2 \longrightarrow 16\,CO_2 + 18\,H_2O}$$ + Reaction energy

An <u>exothermic</u> reaction

Standard Enthalpy of Formation, ΔH_f^0

The change of enthalpy that accompanies the formation of 1 mole of a substance in its standard state from its constituent elements in their standard states

Enthalpies of formation (ΔH_f^0):

C_8H_{18}	: -250 kJ/mol
O_2	: 0 kJ/mol
CO_2	: -394 kJ/mol
H_2O	: -286 kJ/mol

$$H_2 + 1/_2\, O_2 + \text{Energy} \longrightarrow H_2O$$

$$\Delta H_f^0 = -286 \text{ kJ/mol}$$

- The reaction energy (ΔH_{reac}^0) = $\Delta H_f^0{}_{(prod)} - \Delta H_f^0{}_{(start)}$

Example

$$2\, C_8H_{18} + 25\, O_2 \longrightarrow 16\, CO_2 + 18\, H_2O$$

$$\Delta H_{reac}^0 = (((16 \times (-394)) + (18 \times (-286))) - ((2 \times (-250)) + (25 \times 0))) = -10952 \text{ kJ/mol}$$

This equals $-10952/(2 \times M_{C_8H_{18}} + 25 \times M_{O_2}) = -10.6$ kJ/g propellant

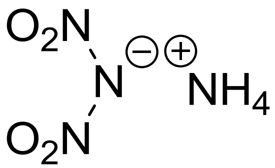
Part 2: Calculating Propellant Performance

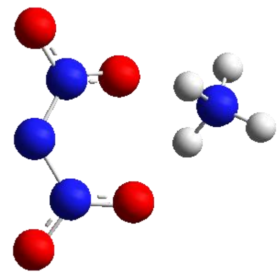
Bond-dissociation energy, BDE (kJ/mol)	
C-C	347
C-H	413
H-H	432
O-H	467
O=O	495
C=O	745
N-H	391
N≡N	941

Standard enthalpy of formation, ΔH_f^0 (kJ/mol)	
Aluminium, Al(s)	0
Aluminium oxide, Al_2O_3(s)	-1676
Ammonium dinitramide (ADN), $NH_4N(NO_2)_2$(s)	-148
Ammonium perchlorate, NH_4ClO_4(s)	-296
Carbon dioxide, CO_2(g)	-394
Nitrogen, N_2(g)	0
Dinitrogen tetroxide, N_2O_4(l)	-20
Methyl hydrazine, CH_6N_2(l)	54
Hydrochloric acid, HCl(g)	-92
Oxygen, O_2(g)	0
Water, H_2O(l)	-286
Hydrogen, H_2(g)	0

Ammonium Dinitramide (ADN)

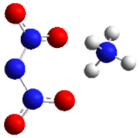
An environmentally friendly oxidant for use in rocket propellants?



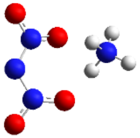


$$3\ NH_4N(NO_2)_2 + 4\ Al \longrightarrow 2\ Al_2O_3 + 6\ N_2 + 6\ H_2O$$

- An energetic molecule free of chlorine
- Discovered in the former Soviet Union in the 1970:s. Possibly used in intercontinental nuclear missiles.
- Rediscovered in the US in the late 80:s. Since then subject of intense research.



Ammonium Dinitramide (ADN)



- Main component of an environmentally friendly liquid propellant in satellites (LMP-103S)
- Developed in Sweden (FOI, ECAPS, EURENCO Bofors)
- Problematic behavior in the solid state
- Incompatible with commonly used plastic binders
- Quantum chemical calculations have contributed to an increased understanding of ADN’s chemistry

Photo: NASA

Quantum Chemical Calculations

- Has revolutionized chemical research over the last decade
- Used in nearly all areas in chemistry
- Organic chemistry: Predicting chemical reactions
- Biochemistry: Studying substrate-protein interactions
- Inorganic and Physical chemistry: Predict and explain structure and bonding
- Materials chemistry: Investigate and design material properties
- Pharmaceutical companies: Theoretical design and investigation of drugs

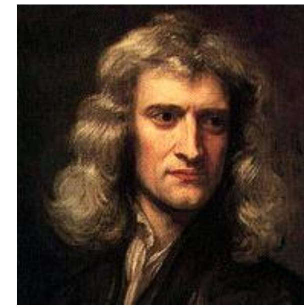
Quantum Mechanics/Chemistry – Theory

- Classical mechanics does not apply to small systems
- Quantum mechanics: a molecular system can be completely described by its wave function, Ψ
- The wave function is obtained from the Schrödinger equation

The Hamiltonian → $\hat{H}\Psi = E\Psi$ ← Wave function

System energy

- Solved in an approximate way for systems consisting of more than two particles



Isaac Newton 1642-1727

Erwin Schrödinger 1887-1961

Quantum Mechanics/Chemistry – Theory

$$\hat{H}\Psi = E\Psi$$

- To obtain the energy, we apply the Hamiltonian operator onto the wave function

$$\hat{H} = -\boxed{\sum_{i=1}^{N}\frac{1}{2}\nabla_i^2} - \boxed{\sum_{A=1}^{M}\frac{1}{2\mu_A}\nabla_A^2} - \boxed{\sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}}} + \boxed{\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}}} + \boxed{\sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{r_{AB}}}$$

Kinetic energy electrons

Kinetic energi nuclei

Attraction electron-nucleus

Repulsion electron-electron

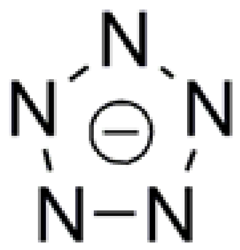
Repulsion nucleus-nucleus

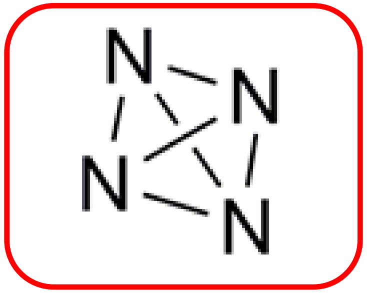
Quantum Chemical Methods

- Semi-empirical methods (*e.g*. PM3)
  - Simplified form of the Hamiltonian
  - Requires less computational power
  - Can be used to obtain geometries. Too innacurate for reliable energies.

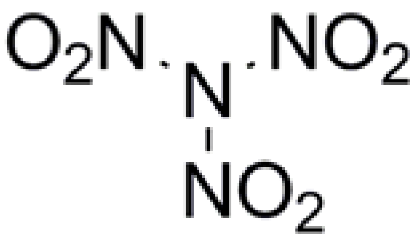
- Density Functional Theory (DFT)
  - Advanced calculations with much less severe approximations
  - Highly accurate energies

Possible Environmentally Friendly Candidates

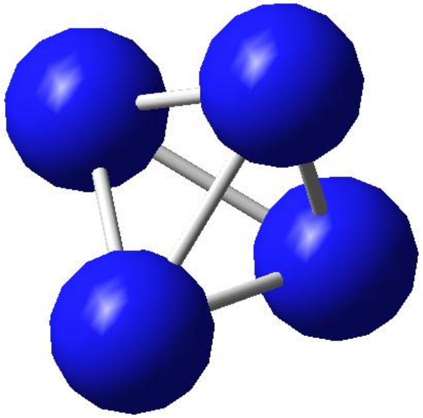




N_4



N_4 – The Optimal Rocket Propellant?



Part 3: Computational Modelling Exercise

- Investigate if tetrahedral N_4 can exist and the amount of energy that would be formed upon its conversion into two N_2
- Start the computer, open HyperChem and follow your handouts

Summary

- Space shuttle propellants have a negative impact on the environment
- Energy is released through rearrangements of chemical bonds
- Thrust is generated when gases accelerate through the nozzle
- Enthalpies of formation can be used estimate propellant energy content
- Ammonium dinitramide (ADN) – an environmentally friendly oxidant
- Computer modelling helps us to find promising new alternatives

Part 4: Testing the Model Rocket Engine

Here we show a more zoomed-in movie in slow motion of when we launch the model rocket using the model rocket engine. The movie file is provided online in the supporting information section.