Chem 1B Objective 11:

Predict heat and work in physical and chemical reactions.

<u>Key Ideas</u>: Energy is involved in every physical and chemical process. Use in heating or cooling. See hot and cold packs. Chem 1A: Heat = amount of energy transferred due to a difference in T Heat gained by cold object = - heat lost by hot object Physical heat transfer: q = ms Δ T Chemical heat transfer: q = Δ H Calculate Δ H using Hess' law: Δ H = Σ n Δ Hf (products) – Σ n Δ Hf (reactants)

Gases are compressible so you can use gas expansion to produce work or you have to supply work to compress a gas. Work = w = -p ΔV

1st law of thermodynamics: $\Delta E = q + w$

Every Chemical Reaction or Physical Process Involves Energy

Energy is "_____"

How fast/slow is reaction?	Does reaction occur?
Reaction Rate (Kinetics) deals with substances (intermediates) that form as reactants go to products.	Thermodynamics deals with reactants (initial state) and products (final state).
3 Factors:	2 Driving Forces:
Concentration	Enthalpy
Temperature	Entropy
Catalyst	



Which part of the reaction energy diagram gives you information about thermodynamics? Which part of the reaction energy diagram gives you information about kinetics?

Thermochemistry (CHM 1A) Involves Heat

a. Is heat the same as temperature? (i) yes (ii) no

b. What are the 3 factors that determine the amount of heat transferred?(i) temperature (ii) time (iii) mass (iv) specific heat

c. A rock and gold cup lie in the middle of a parking lot on a hot day. Which object contains more heat?
(i) rock (ii) gold cup (iii) neither (iv) both

d. How is ΔH calculated?

(i) very carefully (ii) Hess' law (iii) guess

<u>Heat</u> (q)

is the amount of energy transferred from one object to another due to a difference in temperature.

Heat gained by cold object = - Heat lost by hot object (endothermic) (exothermic)

Physical Heat transfer: $q = m s \Delta T$

Chemical Heat transfer: $q = \Delta H$

 ΔH is calculated from Hess' law

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Physical Heat transfer: $q = m s \Delta T$



http://www.huladaddy.com/ articles/coffee-burns.htm Your hot coffee is too hot so you pour 20 ml of cold (25°C) water into your 1 cup (240 ml) of hot (70°C) coffee (assume H_2O).

What is the new (final) temperature of coffee?

Physical Heat transfer: $q = m s \Delta T$

3 factors affect q:

<u>Mass</u>: amount of substances in contact with each other <u>Specific heat</u>: energy needed to raise T of 1 g of substance 1°C <u>Temperature</u>: how hot and cold substances are



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Heat gained by cold $H_2O = -$ Heat lost by hot coffee (endothermic) (exothermic)

Physical Heat transfer: $q = m s \Delta T$

 $m_{\text{cold water}} s_{\text{cold water}} (T_{\text{f}} - T_{\text{i cold water}}) = -m_{\text{hot water}} s_{\text{hot water}} (T_{\text{f}} - T_{\text{i hot water}})$

(20 g) (4.18 J/g °C)($T_f - 25^{\circ}C$) = -(240 g)(4.18 J/g °C)($T_f - 70^{\circ}C$)

Solve for T_f = 66.5°C. Will you need to add more cold water?

A Fuel Contains Energy That Energy is Released when the Fuel Burns Fuel + $O_2 \rightarrow CO_2 + H_2O$ Lab 7 Energy Content and Work in Foods

Part A. Determine the energy content in a food

How to Measure ∆H?



Heat Gained by water (physical Heat Transfer)

Burn the food! Food + $O_2 \rightarrow CO_2 + H_2O$



Heat Lost by food burning (chemical heat transfer)

http://www.rsc.org/learn-chemistry/resource/ res00000397/energy-values-of-food? cmpid=CMP00000467

"A Chemical Reaction Occurs When Reactant Atoms/ Molecules Collide with Sufficient Energy for Bonds to Break or Form."

When a bond is broken, energy is _____.

When a bond is formed, energy is _____.



http://www.reddit.com/r/Fitness/comments/2ysdl7/bench press do you need to be actively flexing/



"A Chemical Reaction Occurs When Reactant Atoms/ Molecules Collide with Sufficient Energy for Bonds to Break or Form." Hydrogen - Fuel of the 21st Century?!

http://www.blewbury.co.uk/energy/hydrogen.htm

Objective: Determine HEAT GAINED/LOST in a chem reaction

E.g., 2 H₂ (g) + O₂ (g) ---> 2 H₂O (g)

H-H O=O H-O-H

2 H-H bonds breaks = energy <u>supplied</u> (endothermic)
1 O=O bond breaks = energy <u>supplied</u> (endothermic)
4 H-O bonds form = energy released (exothermic)

HEAT GAINED/LOST depends on how much energy is supplied compared to how much energy is released.

To Break a Bond **REQUIRES** Energy When a Bond Forms, Energy is **RELEASED**

Bond	ΔH, kJ/mole	Bond	ΔH , kcal/mole
H-H	432	0-Н	459
0-0	142	O=0	494

http://www.wiredchemist.com/chemistry/data/bond_energies_lengths.html

$$2 H_2 (g) + O_2 (g) ---> 2 H_2 O (g)$$

H-H O=O H-O-H
2 H-H bonds breaks = 432 kJ x 2 supplied = 864 kJ
1 O=O bond breaks = 494 kJ supplied = 494 kJ
4 H-O bonds form = 459 kJ x 4 released = -1836 kJ
TOTAL (Net Energy) = -478 kJ
Exothermic

HEAT GAINED/LOST depends on how much energy is supplied compared to how much energy is released.



"A Chemical Reaction Occurs When Reactant Atoms/ Molecules Collide with Sufficient Energy for Bonds to Break or Form."

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Chem 1A!

Objective: Determine HEAT GAINED/LOST using Hess' law

E.g., $2 H_2 (g) + O_2 (g) ---> 2 H_2 O (g)$ ΔH_f , kJ/mole 0 0 -241.8Hess' law: $\Delta H = \Sigma n \Delta H_f$ (products) - $\Sigma n \Delta H_f$ (reactants) $= [2 \times (-241.8)] - [2 \times 0 + 1 \times 0]$ = -483.6 kJ ===> EXOTHERMIC

This means 483.6 kJ of energy is released when 2 moles of H_2 burns.



Hess' law: $\Delta H = \Sigma n \Delta H_f$ (products) - $\Sigma n \Delta H_f$ (reactants) Compare the following fuels: CH₄, C₂H₆, C₃H₈, C₄H₁₀, C₆H₁₄, C₈H₁₈, C₂H₅OH, MTBE, and H₂. Based on ΔH_f , <u>which fuel produces the most heat</u>?

Fuel	ΔH_{f} , kJ/mole
H ₂	0
CH ₄	-74.8
C_2H_6	-84.8
C_3H_8	-103.8
C_4H_{10}	-126.5
C ₆ H ₁₄	-198.8
C_8H_{18}	-250.2
C ₂ H ₅ OH	-278
MTBE	-315

 ΔH_{f} = enthalpy of formation

<u>Formation reaction</u>: substance formed from its elements in standard state

E.g., formation of CH_4 (g) C (s) + 2 H₂ (g) --> CH_4 (g)

Table. Heats of Combustion of Various Fuels

Fuel	Molar mass	∆H _{combustion} , kJ/mole	$\Delta H_{combustion}$, kJ/ mole of C	$\Delta H_{combustion}, kJ/g$
H ₂	2	-285		-143
CH ₄	16	-802	-802	-50.1
C_2H_6	30	-1428	-714	-47.6
C ₃ H ₈	44	-2044	-681	-46.5
$C_{4}H_{10}$	58	-2656	-642	-45.8
C ₆ H ₁₄	86	-3855	-634	-44.8
C ₈ H ₁₈	114	-5074	-634	-44.5
C ₂ H ₅ OH	46	-1234	-617	-26.8
MTBE	86	-3103	-621	-35.3

Hydrogen - Fuel of the 21st Century?!

Objective: Use Chemical Reaction To Heat Something

E.g., Calculate the mass of water that can be heated from 25° C to 100° C by burning 1 g of H₂.

2 H₂ (g) + O₂ (g) ---> 2 H₂O (g) ∆H = - 483.6 kJ for 2 moles.

Heat gained by cold H2O = - Heat lost by H2 burning reaction
(endothermic)(exothermic)Physical heat transferChemical heat transfer

(x g) (4.18 J/g °C)(100°C - 25°C) = -(1 g)(-483,600 J)(1 mole)(2 moles) (2 g)

Solve for $x = _{390 g}$

Identify each phase change as exothermic or endothermic:

- Evaporation
- Condensation
- Melting
- Freezing

What's Going On Here?



http://k9recreation.com/cooling-stations.php

The temperature inside your kitchen oven is 350°F. How can you use a bowl of water to lower the temperature inside the oven?



http://www.123rf.com/photo_10143522_empty-plate-insideelectric-oven-ready-for-food.html



Explain how sweating cools you off.

http://www.sweatblock.com/5myths-about-sweat/

Explain how a swamp cooler works.

http://opalcat.com/Information/swampcoolers

Use this idea to make a solar refrigerator



Identify each phase change as exothermic or endothermic: Evaporation Condensation Melting Freezing

You heat up 1 cup (240 ml) of water from 25°C to 125°C. What happens to the temperature at the boiling point? Draw a heating curve.

Calculate q.

You heat up 1 cup (240 ml) of water from 25°C to 125°C. What happens to the temperature at the boiling point? Draw a heating curve.

Calculate q.

<u>3 Steps</u>: 1. H_2O (I) at 25°C ---> H_2O (I) at 100°C 2. H_2O (I) at 100°C ---> H_2O (g) at 100°C 3. H_2O (g) at 100°C ---> H_2O (g) at 125°C specific heat of steam = 2.0 J/g°C Use: $q_1 = m \le \Delta T$ $q_2 = \Delta H$ $q_3 = m \le \Delta T$

Answer:
$$q_1 = 75,240 \text{ J}, q_2 = 587,000, q_3 = 3750 \text{ J}$$

 $q_{total} = 666,000 \text{ J}$

What is Worse?



Burned by $H_2O(g)$ ORBurned by $H_2O(I)$ at 100°C?at 100°C

https://healthnbodytips.com/health-benefits-of-drinking-hot-water-drink-hot-water-with-honey-and-lemon.html/

Lab 7, Part B Basic Rocket Science



Chem 1B Lab – Spring 2016 (Courtesy of T. Green)

Bring a 0.5 liter plastic bottle to lab.

Gasoline for our cars

2007: world oil demand = 85 million barrels/day U.S. oil demand = 20 million barrels/day approximately 10 million barrels/day for gasoline 141 billions gallons gas/year SJ Mercury News, 11/9/07: 32 million registered cars in CA California = 16 billion gallons gas/year

Engine friction consumes 10% of a car's or truck's fuel:

≈ 1.4 million barrels of oil wasted per day in U.S.

≈ \$31 billion worth of petroleum lost in automobile engines every year (at \$60 per bbl).

Reduce friction losses ==> significant savings in fuel consumption

Tribology: study of friction (in mechanical engineering field) http://cen.acs.org/articles/88/i41/Fighting-Friction.html

A Car Engine Is A Heat Engine *A Fuel Produces Heat A Fuel Produces Work (Or Not)*



What happens in the hot reservoir? How is heat converted to work? Is all of the heat converted to work? What is the efficiency of an engine?

Heat Engine schematic

What is the source of gas in a car engine? What causes the gas to expand?



A Car Engine Is A Heat Engine *A Fuel Produces Heat A Fuel Produces Work (Or Not)*





http://footage.shutterstock.com/clip-913270-stock-footage-balloon-expandable-stent-

opening-a-clogged-artery-with-a-stent.html

What is the hot reservoir? Is heat produced? Is work produced? Compare the following fuels:

 CH_4 , C_2H_6 , C_3H_8 , C_4H_{10} , C_6H_{14} , C_8H_{18} , C_2H_5OH , MTBE, and H_2 . *Which fuel produces the most work*?

Fuel	ΔH_{f} , kJ/mole
H ₂	0
CH ₄	-74.8
C_2H_6	-84.8
C ₃ H ₈	-103.8
C ₄ H ₁₀	-126.5
C ₆ H ₁₄	-198.8
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C ₂ H ₅ OH	-278
MTBE	-315

What does this picture tell you about work?



http://www.learnthermo.com/T1-tutorial/ch04/lesson-A/pg09.php

Work (4 letter word) is the Ability to Move Matter Physics: $w = f \cdot d$ Chemistry: $w = -p \Delta V$



Work involves Gases

Gas <u>expands</u> ==> $\Delta V > 0$ ==> w < 0Work is produced Work done by gas

Example: an explosion produces work by gas expansion

http://www.learnthermo.com/T1-tutorial/ ch04/lesson-A/pg09.php

Gas *contracts* ==> ∆ V < 0 ==> w > 0 Work is supplied Work done on gas

Example: a compressor supplies work to compress a gas

Diesel engines are more efficient than gasoline engineGasoline engineDiesel engineEfficiency = 20%Efficiency = 35-40%

Diesel engine contains **excess** air during combustion Combustion products expands more and transfers more energy into pushing the piston for same amount of fuel (http://cen.acs.org/articles/94/i23/Start-engines.html)

Diesel engine: higher compression ratio (higher P) ---> higher combustion T

Diesel fuels - linear aliphatic and cycloaliphatic hydrocarbons (higher boiling points) Gasoline fuels - branched aliphatic and aromatic hydrocarbon (lower boiling points) **Objective**: Determine work in a chemical reaction.

When methane (natural gas, CH_4) burns, is work produced? 1. Balance chemical equation:

 $CH_4(g) + 2O_2(g) ---> CO_2(g) + 2H_2O(g)$

Compare moles of gas reactants to moles of gas products
 3 moles of gas reactants ---> 3 moles of gas products

3. Calculate Δ n = moles of gas products - moles of gas reactants

$$\Delta$$
 n = 3 - 3 = 0

4. Calculate w =
$$-p \Delta V = -\Delta n R T$$

 $\Delta n = 0$ so $\Delta V = 0$ so w = 0

Q: Does methane contain work? Q: Is work produced when gasoline, C₈H₁₈, is burned?

Table. Heat and Work Comparison of Fuels

Fuel	∆H, kJ/g	ΔS , J/mole K	Δn	ΔV	W
CH ₄ (g)	-50.1	-5.2	0	0	0
$C_{2}H_{6}(g)$	-47.6		0.5	>0	<0
C ₃ H ₈ (g)	-46.5		1	>0	<0
C ₄ H ₁₀ (g)	-45.8	155.7	1.5	>0	<0
C ₆ H ₁₄ (I)	-44.8	360	3.5	>0	<0
C ₈ H ₁₈ (I)	-44.5	484	4.5	>0	<0
C ₂ H ₅ OH(I)	-26.8	217	1	>0	<0
MTBE (I)	-35.3		2.5	>0	<0
$C_{6}H_{12}O_{6}(s)$	-14.1	972	5	>0	<0
H ₂ (g)	-120.9	-44	-0.5	<0	>0

A Refrigerator Is A Heat Engine in Reverse

Show heat in, heat out, and work.

Energy (Work) Is Supplied To Run A Compressor

Phase Changes Are Involved to Cool Air



c. Describe the phase changes the refrigerant undergoes in a refrigerator cycle.

d. How is air cooled inside the refrigerator? <u>http://www.energyquest.ca.gov/how_it_works/refrigerator.html</u> <u>http://home.howstuffworks.com/refrigerator.htm</u> How Does a Refrigerator Work? http://home.howstuffworks.com/refrigerator3.htm



High P gas

A: Low P gas --> High P gas

B: High P gas --> High P liq

C: High P liq --> Low P liq

D: Low P liq --> Low P gas

a. Determine q and w for each step.

b. Which step cools air inside the refrigerator?

c. Would you want the refrigerant to have a high boiling point or low boiling point? Give reasons.

d. Would you want the refrigerant to be compressible or incompressible? Give reasons.



<u>Natural Gas (fossil fuel) is used for heating and cooking</u> 1 therm = 100,000 Btu = 105.4804 MJ PG&E rate = \$1.30/therm

Calculate the mass of methane burned to produce 1 therm.

Electricity is Used for heating and cooking, lights, etc. 1 kW hr = 3.6×10^6 J = 3.6 MJ = 0.034 therm PG&E rate = 0.24/kW hr

Is Electricity cheaper than Natural Gas?

The 1st Law of Thermodynamics Tells Us Energy Can Be Converted From One Form to Another

What equation tells us the first law of thermodynamics?

 $q_{gained} = - q_{lost}$

temperature mass $q = ms\Delta T$

 $\Delta E = q + w$ Specific heat

pressure

 $\Delta H = \Sigma n \Delta H_f$ (products) - $\Sigma n \Delta H_f$ (reactants)

Describe the conversion of one type of energy into another in:

- 1. Hydroelectric dam
- 2. Battery
- 3. Car engine

Kinetic energy

Electrical energy

Chemical energy

Mechanical energy

Solar energy

Potential energy

Nuclear energy

heat

work

Corn ----> Ethanol as Fuel Chemical Energy ----> Mechanical Energy

US corn: 50% for animal feed, 33% for car fuel, rest exported or processed to produce sweeteners, corn oil, and other products. Rest of world eats corn. (CEN, 9/13/10, p. 20)

There are many companies that are converting corn to ethanol, e.g., Archers Daniels Midland.

a. Calculate the heat of combustion of ethanol in kJ/mole and kJ/g.
Determine the work produced by ethanol in this reaction. Compare this heat and work to that of octane. Which fuel is the better fuel? Give reasons.
b. However, some scientists believe ethanol is not the solution. See
(i) Ethanol Fuel from Corn Faulted as 'Unsustainable Subsidized Food Burning' <u>http://healthandenergy.com/ethanol.htm</u>
(ii) Ethanol can replace gasoline with significant energy savings, comparable impact on greenhouse gases
<u>http://berkeley.edu/news/media/releases/2006/01/26_ethanol.shtml</u>
(iii) Food vs. fuel <u>http://en.wikipedia.org/wiki/Food_vs._fuel</u>
Is ethanol a good alternative to fossil fuels?

MAKING CELLULOSIC BIOFUELS



SOURCES: Energy Information Administration, company information

http://cen.acs.org/articles/91/i4/Building-New-Biofuels-Industry.html

<u>Where does electricity come from?</u> Total Electricity Produced in US = 3.95x10¹² kW hr (2009)

Reference: http://www.eia.gov/totalenergy/data/annual/index.cfm -2009



Where does the electricity come from for an electric car?

http://cen.acs.org/articles/90/i18/Local-Look-PlugVehicles.html 4/30/12, CEN, p. 32 **Do Plug-in Electric Vehicles Make Economic and Environmental Sense?**

Electricity on West coast and parts of the eastern coast comes from a mix of fuel sources. Emissions and operating costs strongly favor electric vehicles. E.g., in California and New York, electric vehicles would be equivalent to a hypothetical gasoline-powered, 80-mpg vehicle in emissions and environmental performance.

Rocky Mountain and midwestern states depend more on coal-fired power plants for electricity. In these states greenhouse gas emissions from electric vehicles will be higher than in other regions, and electric vehicles' performance can match only those of a 33-mpg vehicle.

Vehicles charged in regions that rely more on natural gas than coal to generate electricity will produce less carbon dioxide. If the trend away from coal continues, plug-in vehicles will have the unique distinction among automobiles of producing fewer emissions as they age.

In terms of fuel costs based on electricity rates in 50 U.S. cities, electric-vehicle drivers will spend \$750 to \$1,200 less per year than will drivers operating an average new compact vehicle fueled by gasoline costing \$3.50 per gal.

RESOURCES

Estimates suggest that there are huge quantities of recoverable oil and gas on the U.S. outer continental shelf



CEN, October 3, 2005, pp. 31–34 Rethinking Energy Policy

<u>Hydraulic Fracturing</u> (Fracking) pumps millions of gallons of treated water and sand into the ground at extremely high pressure to generate fractures or cracks in shale rocks to release natural gas.

Year	% of U.S. natural gas from shale rock
2000	1
2010	20
2035	50

"Most significant energy innovation of this century"

U.S. now has about 2,074 trillion cu ft of technically recoverable natural gas resources—enough to meet domestic demand for more than a century at the current rate of consumption.

http://cen.acs.org/articles/88/i22/Drilling-Process-Draws-Scrutiny.html



http://cen.acs.org/articles/90/i42/Treating-Water-Hydraulic-Fracturing.html

FRACKING RECIPE

Example of fracturing fluid composition from a gas well in Beaver, Pa.

INGREDIENT FUNCTION	CHEMICAL	MAXIMUM INGREDIENT CONCENTRATION, % BY MASS
Carrier/base fluid	Freshwater	85.47795%
Proppant	Crystalline silica	12.66106%
Acid	Hydrochloric acid in water	1.29737%
Gelling agent	Petroleum distillate blend	0.14437%
	Polysaccharide blend	0.14437%
Cross-linker	Methanol	0.04811%
	Boric acid	0.01069%
Breaker	Sodium chloride	0.04252%
Friction reducer	Petroleum distillate, hydrotreated light	0.01499%
pH-adjusting agent	Potassium hydroxide	0.01268%
Scale inhibitor	Ethylene glycol	0.00540%
50	Diethylene glycol	0.00077%
Iron control agent	Citric acid	0.00360%
Antibacterial agent	Glutaraldehyde	0.00200%
	Dimethyl benzyl ammonium chloride	0.00067%
Corrosion inhibitor	Methanol	0.00142%
Ale 3%	Propargyl alcohol	0.00010%

NOTE: Additional proprietary ingredients not listed in material safety data sheet: acid, alcohol, biocide, copolymer, disinfectant, enzyme, polymer, silica, solvent, surfactant, and weak acid. **SOURCE:** FracFocus

Currently, on a global scale, **energy usage is on the order of 13 terawatts** (13 trillion W or 13 trillion joules per second), of which roughly **85% is generated by burning fossil fuels**. (CEN, 8/27/07, p. 16)



"MORE ENERGY—in the form of sunlight—strikes Earth in one hour than all of the energy consumed by humans in an entire year." -- Nathan Lewis, Cal Tech Chemistry Professor

Sun showers Earth with an energy flow of some 120,000 TW.

We need to Figure out a way to *inexpensively* convert sunlight to electricity.

Solar Energy ≈ 0.125% of U.S. electricity (2008) CEN, 10/20/08, p. 40 920 MW on Electric Grid = 500 MW photovoltaics + 420 MW concentrating solar power 2260 MW captured solar from solar calculators, road signs, pools,



Polysilicon solar cells 14% efficiency http://www.topsky-tech.com/poly-siliconsolar-cell-tianwei-supplier.html Thin Films 8% efficiency http://www.circuitstoday.com/thinfilm-solar-cell

http://cen.acs.org/articles/90/i23/Shade-Hot.html

Dye-Sensitized Solar Cells (DSSC) generate electricity from light by mimicking photosynthesis. Efficiency = 26%. Use ambient indoor light. Use to replace disposable batteries? DSSC consists of a film of inexpensive porous TiO_2 nanoparticles coated with a sunlight-absorbing dye, often a ruthenium compound, in contact with a liquid electrolyte solution.



http://cen.acs.org/articles/90/i24/Solid-Solar-Cell-Solution.html (CEN, 6/11/12) Solid Solar-Cell Solution New solid electrolyte bypasses corrosion and durability problems of traditional dye-sensitized solar cells