Introduction to

Thermodynamics

Heat (Chemical Energy) in Physical & Chemical Changes

Principles, Equations & Diagrams

Dr. Ron Rusay

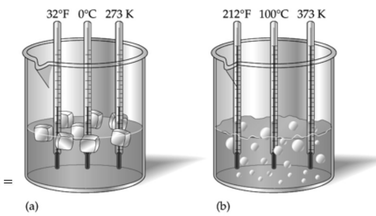
UNITS: Celsius (°C) & Kelvin (K)

Temperature is **NOT ENERGY**

"**Temperature** (sometimes called thermodynamic **temperature**) is a measure of the average kinetic energy of the particles in a system. Adding heat (energy) to a system causes its **temperature** to rise."

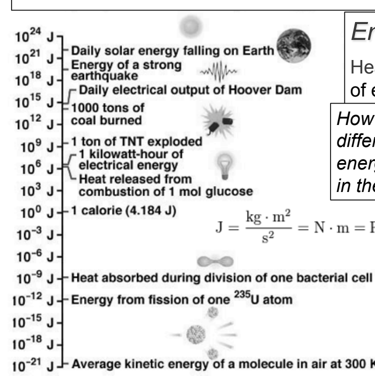
August. 15, 2015
+142°F Manama, Bahrain

°C? = 61.7°C
K? = 61.7°C +273.15 = 334.85 K



Kinetic Energy One of Many Types of Energy

- *Kinetic Energy is due to the motion of an object.*
  - *KE = ½ mv²*
  - *(m = mass, v = velocity)*



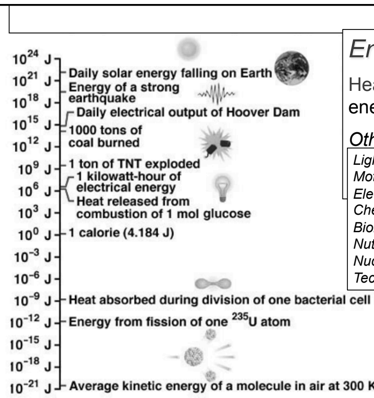
Energy:

Heat is one form of energy.

How many other different types of energy are included in the graphic?

$$J = \frac{kg \cdot m^2}{s^2} = N \cdot m = Pa \cdot m^3 = W \cdot s = C \cdot V$$

UNITS:
m = meter
joule (J)
calorie (c)
kilocalorie (C)
Kilowatt hour (kWh)



Energy:

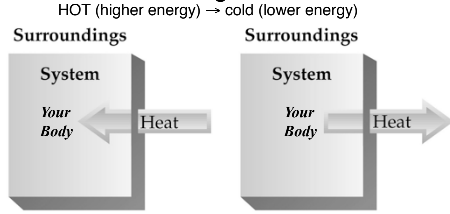
Heat, one form of energy.

Others:

Light (solar/radiant)
Motion (kinetic)
Electrical
Chemical
Biological
Nutritional (Food)
Nuclear
Tectonic

Thermoregulation

HOT (higher energy) → cold (lower energy)

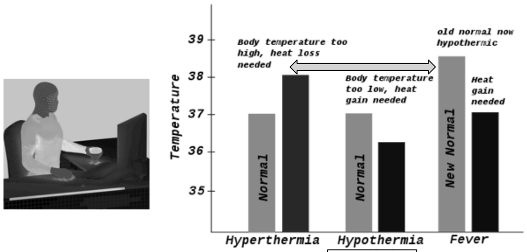


Thermoregulation balance involves the heat transfer to *or* from your body, ***and*** to *or* from the surroundings

Your "Body Mass" is important to Thermoregulation; subcutaneous adipose tissue (fat) provides an insulating layer that impedes heat loss. This can be an advantage or a disadvantage depending on the surroundings. Do you know your Body Mass Index? See the NIH link below:

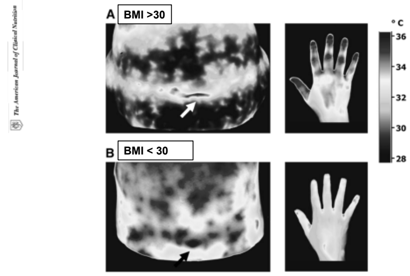
http://www.nhlbi.nih.gov/health/educational/lose_wt/BMI/bmi-m.htm

Thermoregulation: heat transfer to *or* from your body, ***and*** to *or* from the surroundings



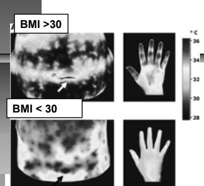
Fever is a temperature above your normal temperature due to an increase in the body's temperature set-point. ***Hyperthermia*** is an increase in body temperature over your temperature set-point, due to either too much heat production or not enough heat loss. ***Hypothermia*** is a decrease in body temperature over your temperature set-point, due to too much heat loss.

Abdominal and hand thermograms of a BMI >30 female (A) and a BMI <30 female (B).

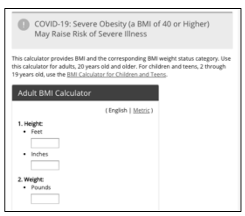


David M Savastano et al. Am J Clin Nutr 2009;90:1124-1131

Increased heat production is associated with BMI >30;
To regulate body temperature, those individuals must increase their heat dissipation through their hands.



Centers for Disease Control
BMI Calculator

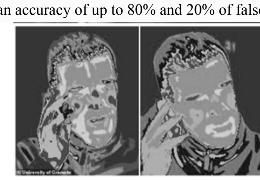


https://www.cdc.gov/healthyweight/assessing/bmi/adult_bmi/english_bmi_calculator/bmi_calculator.html

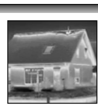
Lying & Temperature Effects (2018)
Dr Emilio Gómez Milán
University of Granada

The so-called 'Pinocchio Effect', which causes the temperature of the nose to decrease between 0.6 ºC and 1.2 ºC while that of the forehead increases between 0.6 ºC and 1.5 ºC when a person is lying.

The new method for detecting lies in a laboratory is more accurate and yields less false positives than a polygraph: it offers an accuracy of up to 80% and 20% of false positives.



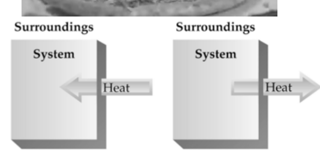
Heat Exchange
Exo- and Endo- thermic Processes & Reactions
(Exergonic and Endergonic)



reactant(s) ⟶ product(s)

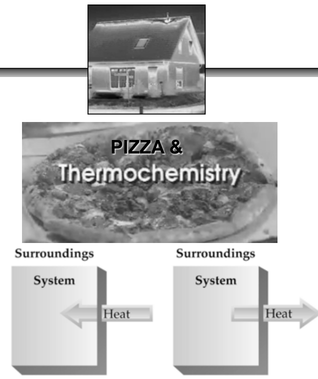
Two types of thermochemical reactions:

- *Exothermic: Heat is a reaction **product;** the heat flows to the surroundings. The amount is the difference between the products minus the reactants. …It is a negative value for the reaction.*
- *Endothermic: Heat is a **reactant;** the heat flows from the surroundings. The amount is the difference between the products minus the reactants…It is a positive value for the reaction.*



Why can you burn the top of your mouth with hot pizza just out of the oven and not the bottom?
(The top & bottom are at the same temperature!!!)

http://chemconnections.org/general/movies/Pizza-thermo%202.mp4



http://www.eia.gov/energyexplained/

Specific Heat Capacities

Substance	Specific Heat Capacity (J/g · K)*
Elements	
Aluminum, Al	0.900
Graphite, C	0.711
Iron, Fe	0.450
Copper, Cu	0.387
Gold, Au	0.129
Compounds	
Ammonia, $NH_3(l)$	4.70
Water, $H_2O(l)$	4.184
Ethyl alcohol, $C_2H_5OH(l)$	2.46
Ethylene glycol, $(CH_2OH)_2(l)$	2.42
Carbon tetrachloride, $CCl_4(l)$	0.862
Solid materials	
Wood	1.76
Cement	0.88
Glass	0.84
Granite	0.79
Steel	0.45

*At 298 K (25°C).

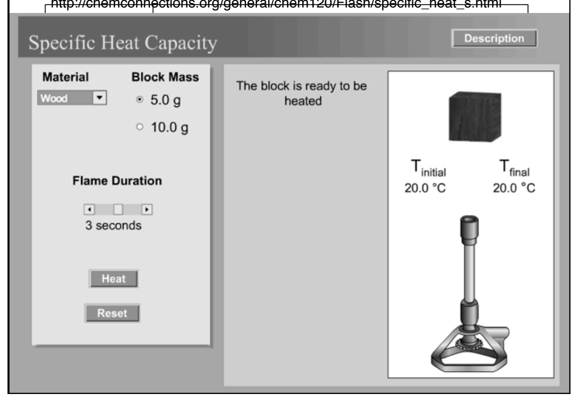
Cp UNITS:
J/(g · K)
or
J/(mol · K)

Energy :
joule (J)
calorie (c)
kilocalorie (C)
Kilowatt hour (kWh)

Chemical
Nuclear
Electrical
Light (solar)
Motion (kinetic)

(Cp) Body fat: In obese mice (fat content 52.76% body wt) the heat capacity is **3.66** kJ kg-1 K-1 and in lean mice (fat content 7.55% body wt) the heat capacity is **2.65** kJ kg-1 K-1.

Specific Heat Interactive Simulation
http://chemconnections.org/general/chem120/Flash/specific_heat_s.html



QUESTION

The specific heat capacity of a sample that was claimed to be gold was determined. It required 48.8 J to raise the temperature of 15 grams of sample 25°C. Is the sample gold? (Use the value in the table on the previous slide, 0.13 J/g°C, for comparison.)

A. YES
B. NO
C. Cannot determine from the data.

Answer

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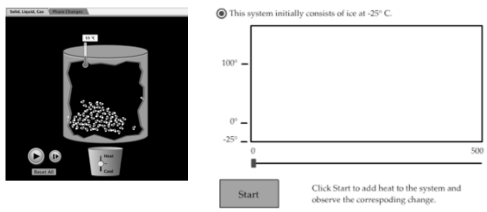
A. YES
B. NO
C. Cannot determine from the data.

0.13 J/g°C = 48.8 J / 15 grams · 25°C

Substance	Specific Heat J / °C · g
$H_2O_{(l)}$	4.18
$H_2O_{(s)}$	2.03

https://phet.colorado.edu/en/simulation/states-of-matter-basics



http://chemconnections.org/general/movies/HeatingCurves.swf

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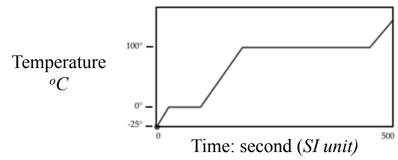
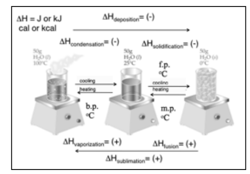
Temperature and Physical States

s ⇆ l ⇆ g

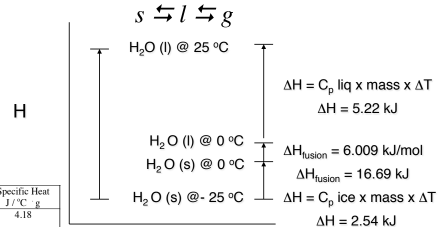




Energy Diagram

Heat @ constant Pressure (Enthalpy) ΔH

s ⇆ l ⇆ g



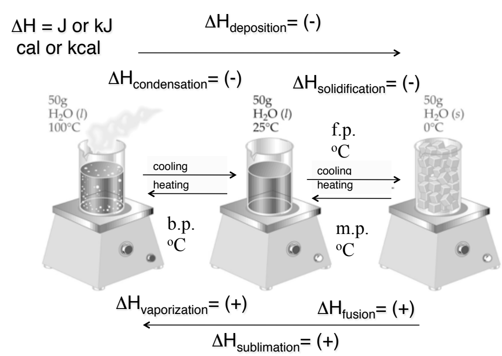
Substance	Specific Heat J / °C · g
$H_2O_{(l)}$	4.18
$H_2O_{(s)}$	2.03
$Al_{(s)}$	0.89
$Fe_{(s)}$	0.45

Process Path $\Delta H = \Delta H_{ice} + \Delta H_{fusion} + \Delta H_{liq}$

If 50.0 g of ice @ -25 °C warms to 25 °C what is ΔH of the process?

ΔH = ?

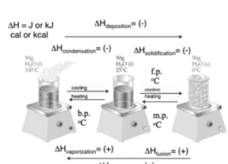
ΔH = 24.45 kJ



QUESTIONs

Answer either: A) endothermic, or: B) exothermic for each of the following 5 changes of physical state.

1. Fusion
2. Vaporization
3. Condensation
4. Sublimation
5. Liquid → Solid



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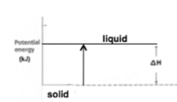

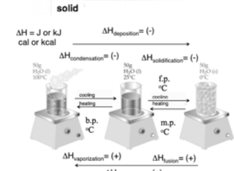

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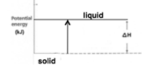
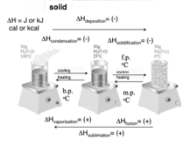
A) endothermic
ΔH_{fusion}= (+)





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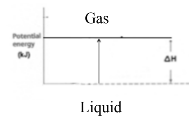

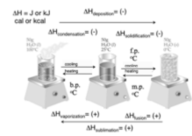

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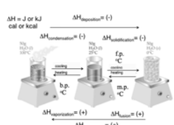
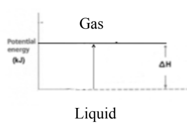
A) endothermic
$\Delta H_{vaporization}$= (+)





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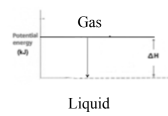

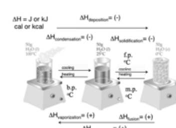

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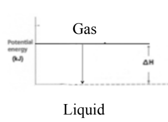
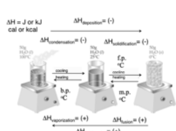
B) exothermic
$\Delta H_{condensation}$= (-)





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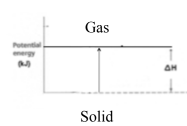

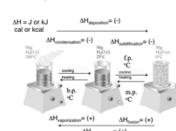

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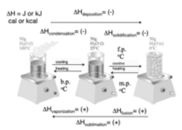
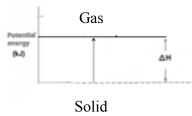
5. Liquid → Solid

A) endothermic

$\Delta H_{vaporization} = (+)$ $\Delta H_{fusion} = (+)$

$\Delta H_{sublimation} = (+)$

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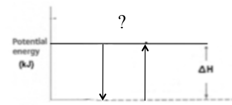

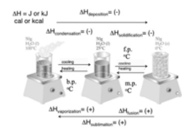

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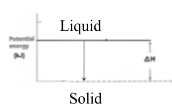
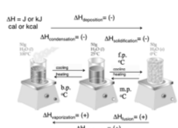
5. Liquid → Solid

B) exothermic
$\Delta H_{solidifcation} = (-)$

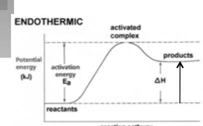


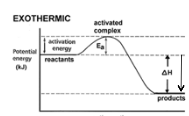


Heat of Reaction

The heat of any reaction can be calculated from the heat(s) of formation of products minus reactants.

$$\Delta H_{rxn}^\circ = \Sigma n_p \Delta H_f^\circ(products) - \Sigma n_r \Delta H_f^\circ(reactants)$$

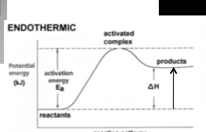


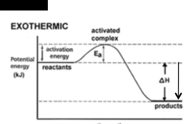


Endothermic $\Delta H_{rxn}^\circ = (+)$ and Exothermic $\Delta H_{rxn}^\circ = (-)$

Heat of Reaction

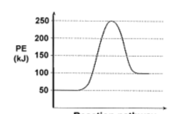
Biological Reactions & Enzyme Catalysts





Endergonic $\Delta H_{rxn}^\circ = (+)$ and Exergonic $\Delta H_{rxn}^\circ = (-)$

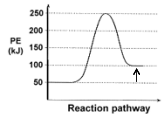
QUESTION



(True/False) The above energy diagram represents an exothermic reaction.

A. TRUE
B. FALSE

Answer



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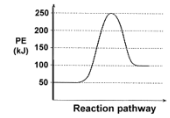
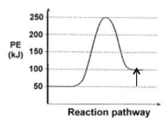


The heat of reaction represented in the above energy diagram is: ________ and is ___________ .

A. +200 kJ and is endothermic
B. -200 kJ and is exothermic
C. +50 kJ and is endothermic
D. -50 kJ and is endothermic
E. -150 kJ and is exothermic

Answer



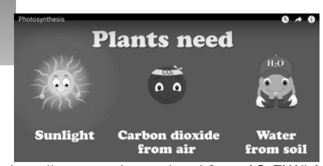
The heat of reaction represented in the above energy diagram is: ________ and is ___________ .

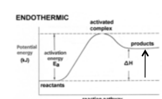
A. +200 kJ and is endothermic
B. -200 kJ and is exothermic
C. +50 kJ and is endothermic
D. -50 kJ and is endothermic
E. -150 kJ and is exothermic

Endothermic Reactions

Photosynthesis

$6\ CO_{2\,(g)} + 6\ H_2O_{(l)} + energy \rightarrow C_6H_{12}O_{6\,(s)} + 6\ O_{2(g)}$





https://www.youtube.com/watch?v=eaACsEXAjhA

$\Delta H_{rxn}° = \Sigma n_p \Delta H_f°(products) - \Sigma n_r \Delta H_f°(reactants)$

$\Delta H_{rxn}° = (+) = +\ 2800$ kJ/mol $C_6H_{12}O_6$ *(glucose or fructose)*

(Enthalpy ΔH)

Endothermic Reactions

$Ba(OH)_2 \cdot 8H_2O(s) + 2NH_4Cl(s) \rightarrow 2NH_3(g) + 10H_2O(l) + BaCl_2(s)$

http://chemconnections.org/general/movies/EndotermHMVID12.MOV

$\Delta H_{rxn}° = \Sigma n_p \Delta H_f°(products) - \Sigma n_r \Delta H_f°(reactants)$

$\Delta H_{rxn}° = (+) = +\ ?$ kJ/mol

QUESTION

Determine the heat of reaction for the reaction from the video. The respective total heats of formation for the total mass (total moles) of reactants is -3973 kJ and the total products is -3811 kJ. Also, identify if the reaction is exothermic or endothermic.

$Ba(OH)_2 \cdot 8H_2O(s) + 2NH_4Cl(s) \rightarrow 2NH_3(g) + 10H_2O(l) + BaCl_2(s)$

A. 7784 kJ, endothermic
B. -7784, exothermic
C. 162 kJ, endothermic
D. -162 kJ, endothermic
E. 162 kJ, exothermic

Answer

Determine the heat of reaction for the following reaction. The respective total heats of formation for the reactants is -3973 kJ and the total products is -3811 kJ. Also, identify if the reaction is exothermic or endothermic.

$Ba(OH)_2 \cdot 8H_2O(s) + 2NH_4Cl(s) \rightarrow 2NH_3(g) + 10H_2O(l) + BaCl_2(s)$

A. 7784 kJ, endothermic
B. -7784, exothermic
C. 162 kJ, endothermic
D. -162 kJ, endothermic
E. 162 kJ, exothermic

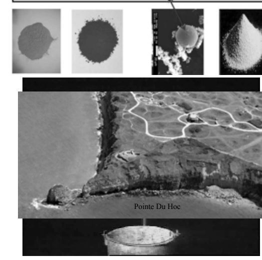
$$\Delta H_{rxn}^\circ = \Sigma n_p \Delta H_f^\circ(products) - \Sigma n_r \Delta H_f^\circ(reactants)$$

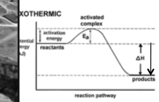
$$\Delta H_{rxn}^\circ = -3811 \text{ kJ} - (-3973 \text{ kJ}) = +162 \text{ kJ/mol}$$

Exothermic Reactions

Fine powder | Fine powder (Rust) | From liquid to Solid Iron Spheres | Fine white dusty powder

$2Al + Fe_2O_3 \xrightarrow[> 450°C]{add\ \Delta} 2Fe(s) + Al_2O_3$



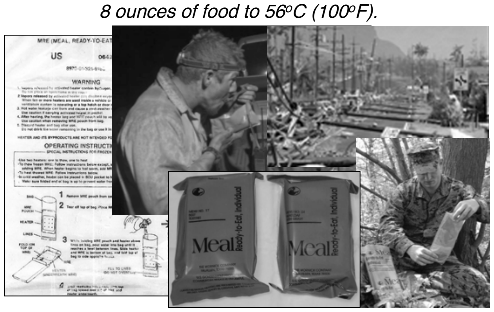


ΔH_{rxn}° = - 14,455 kJ/mol

http://www.youtube.com/watch?v=rdCsbZf1_Ng 1:37

Hot Food: MRE's Exothermic Reaction

Enough heat to raise the temperature of 8 ounces of food to 56°C (100°F).

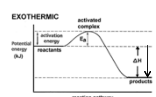


$Mg_{(s)} + 2\ H_2O_{(l)} \longrightarrow Mg(OH)_{2\ (aq)} + H_{2\ (g)}$ + energy:

Exothermic Reactions

Combustion: Burning Carbon Compounds

$C_xH_y + (x + y/4)\ O_2 \rightarrow x\ CO_2 + y/2\ H_2O$ + energy

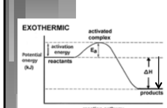


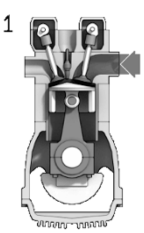
https://www.youtube.com/watch?v=UigjFAI2uWM

Exothermic Reactions

Octane (Gas) Combustion Engine

$2\ C_8H_{18(l)} + 25\ O_{2(g)} \rightarrow 16\ CO_{2(g)} + 18\ H_2O_{(l)}$ + energy





ΔH_{rxn}° = - 5,075 kJ/mol

ΔH_{rxn}° / gallon = ?

1 gallon = 3,785 mL
Density = 0.7 g/mL
1 mole = 114 g/mol
1 gallon C_8 = 23.2 mol C_8

ΔH_{rxn}° / gallon = 118,000 kJ
~ 25 miles
> 18 lbs CO_2

http://chemconnections.org/general/movies/4StrokeEngine_Ortho_3D_Small.gif

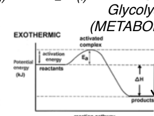
Exothermic Reactions

***Food** / eg. **"Burning" Sugar** → energy*
(Photosynthesis in Reverse)

http://chemconnections.org/general/chem106/Calories-Guide.html

$C_6H_{12}O_{6\ (s)} + 6\ O_{2(g)} \rightarrow 6\ CO_{2\ (g)} + 6\ H_2O_{(l)}$ + energy

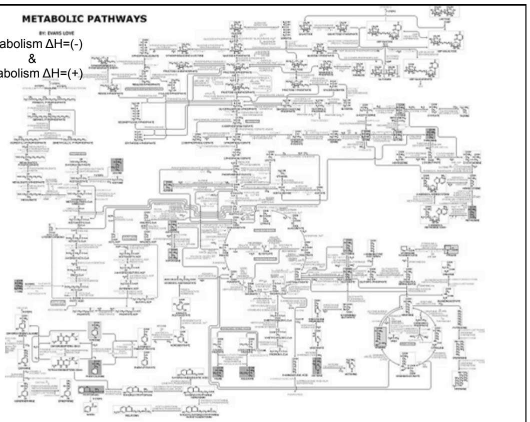
Glycolysis (METABOLISM)



m/watch?v=uWOURkrxpH4

ΔH_f°(reactants)

O_6 (glucose or fructose)

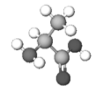
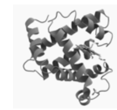


catabolism ΔH=(-)
&
anabolism ΔH=(+)

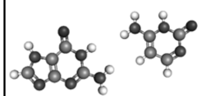
Metabolism:

making & breaking bonds

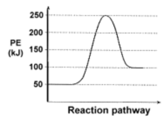
catabolism ΔH=(-)
[breaking down natural polymers]
&
anabolism ΔH=(+)
[building up natural polymers]

Type of molecule	Name of monomer forms	Name of polymer forms	Examples of polymer forms
Amino acids	Amino acids	Proteins (made of polypeptides)	Fibrous proteins and globular proteins
Carbohydrates	Monosaccharides	Polysaccharides	Starch, glycogen and cellulose
Nucleic acids	Nucleotides	Polynucleotides	DNA and RNA



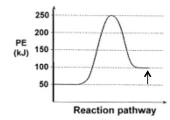

QUESTION



(True/False) Glycolysis is correctly illustrated in the anabolic reaction diagram above.

A. TRUE
B. FALSE

Answer



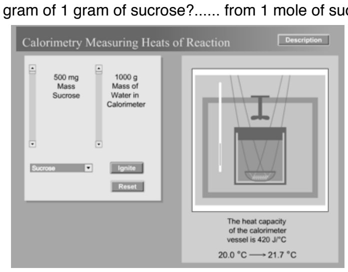
(True/False) Glycolysis is correctly illustrated in the anabolic reaction diagram above.

A. TRUE
B. FALSE

False. Diagram is correct for anabolic reactions (endothermic); glycolysis is an exothermic process.

Calorimetry Interactive

How many kcal of energy (food Calories) do you get from eating (burning) 1 gram of 1 gram of sucrose?...... from 1 mole of sucrose?



m x Cp x ΔT = q (heat)

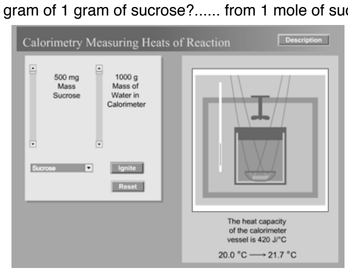
q = ?

http://chemconnections.org/general/chem120/Flash/calorimetry_s.html

$\Delta H_{Reaction}$ = ? kJ /g $_{sucrose}$
$\Delta H_{Reaction}$ = ? kJ /mol $_{sucrose}$

Calorimetry Calculation

How many kcal of energy (food Calories) do you get from eating (burning) 1 gram of 1 gram of sucrose?...... from 1 mole of sucrose?



m x Cp x ΔT = q (heat)

1000. g H_2O x 4.184 J/g°C x (1.7°C) =
= + 7110 J
= + 7110 J + 420 J/°C x (1.7°C)

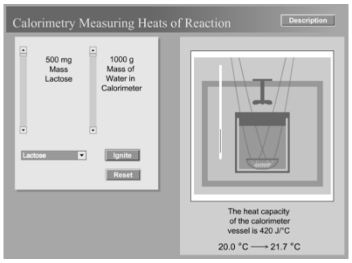
q = -7800 J/ 0.500 g $_{sucrose}$
q = -15600 J / g $_{sucrose}$
q = -15.6 kJ / g $_{sucrose}$
-3.7 Cal /g (kcal /g $_{sucrose}$)

http://chemconnections.org/general/chem120/Flash/calorimetry_s.html

$\Delta H_{Reaction}$ = -15.6 kJ /g $_{sucrose}$ x Molar Mass $_{sucrose}$ [342.3 g/mol]
$\Delta H_{Reaction}$ = -5340 kJ /mol $_{sucrose}$

Comparative Calorimetry

How many kcal of energy (food Calories) can you theoretically get from eating 1/2 gram of lactose versus 1/2 gram of sucrose versus 1/2 gram TNT?



sucrose
ΔT = ?

lactose
ΔT = ?

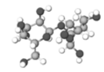
trinitrotoulene (TNT)
ΔT = ?
[dynamite (nitroglycerine) ?]

http://chemconnections.org/general/chem120/Flash/calorimetry_s.html

Bomb Calorimetry (Interactive)

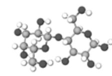
http://chemconnections.org/general/chem120/Flash/calorimetry_s.html

How many kcal of energy (food Calories) can you theoretically get from eating 1/2 gram of lactose versus 1/2 gram of sucrose versus 1/2 gram TNT?



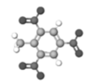
sucrose
$C_{12}H_{22}O_{11}$

$\Delta T = +1.7^oC$



lactose
$C_{12}H_{22}O_{11}$

$\Delta T = +1.7^oC$

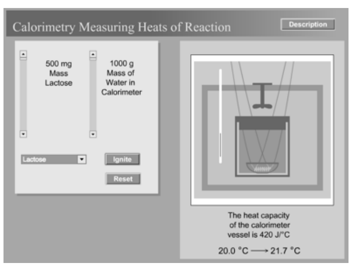


$C_7H_5N_3O_6$

$\Delta T = +1.6^oC$
(Dynamite = 0.7 oC)

Comparative Calorimetry

How many kcal of energy (food Calories) can you theoretically get from eating 1 gram of lactose versus 1 gram of sucrose versus 1 gram TNT?



m x Cp x ΔT = q (heat)

1000. g H_20 x 4.184 J/g°C x (1.7°C) =
= + 7110 J
= + 7110 J + 420 J/°C x (1.7°C)

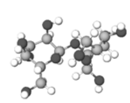
$\Delta H_{Reaction}$ = -15600 J / g

http://chemconnections.org/general/chem120/Flash/calorimetry_s.html

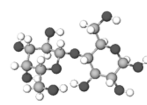
$\Delta H_{Reaction}$ = -15.6 kJ /g $_{sucrose}$ = -3.7 kcal /g $_{sucrose}$
= -15.6 kJ /g $_{lactose}$ = -3.7 kcal /g $_{lactose}$

Bomb Calorimetry (Interactive)

How many kcal of energy (food Calories) do you get from eating 1 gram of lactose versus 1 gram of sucrose?



sucrose
$C_{12}H_{22}O_{11}$



lactose
$C_{12}H_{22}O_{11}$

m x Cp x ΔT = q (heat)

1000. g H_20 x 4.184 J/g°C x (1.7°C) =
= + 7100 J
= + 7100 J + 420 J/°C x (1.7°C)

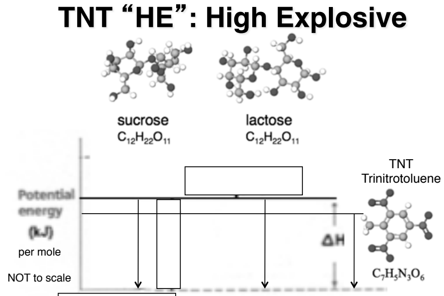
$\Delta H_{Reaction}$ = -7800 J / 0.500 g $_{sucrose}$
$\Delta H_{Reaction}$ = -15600 J / g $_{sucrose}$

http://chemconnections.org/general/chem120/Flash/calorimetry_s.html

$\Delta H_{Reaction}$ = -15.6 kJ /g $_{sucrose}$ = -3.7 kcal /g $_{sucrose}$ = -5340 kJ /mol $_{sucrose}$
= -15.6 kJ /g $_{lactose}$ = -3.7 kcal /g $_{lactose}$ = -5340 kJ /mol $_{lactose}$

How many kcal of energy (food Calories) can you theoretically get from eating 1 gram of lactose versus 1 gram of sucrose versus 1 gram TNT?

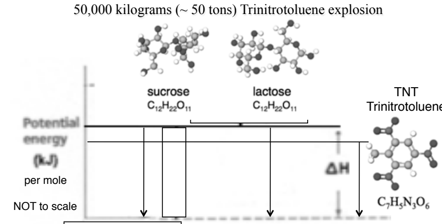
TNT "HE": High Explosive



$\Delta H_{Reaction}$ = -14.2 kJ /g $_{TNT}$ x 227.13 g·mol^{-1}= -3,225 kJ /mol $_{TNT}$
versus -5340 kJ /mol $_{sucrose\ or\ lactose}$

TNT "HE": High Explosive

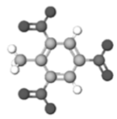
https://www.youtube.com/watch?v=3G3kh39oDPo
400 grams (< 1lb) Trinitrotoluene explosion
https://www.youtube.com/watch?v=zhTiRYwJqHY
5 kilograms (~ 10 lb) Trinitrotoluene explosion
https://www.youtube.com/watch?v=bIQr62lZbsM
50,000 kilograms (~ 50 tons) Trinitrotoluene explosion



$\Delta H_{Reaction}$ = -14.2 kJ /g $_{TNT}$ x 227.13 g·mol^{-1}= -3,225 kJ /mol $_{TNT}$
500,000 kilograms (~ 500 tons) Trinitrotoluene explosion

What makes TNT "explosive" versus sucrose or lactose?

TNT
Trinitrotoluene

_4_  + _21_ 

$$4\ C_7H_5N_3O_6 \quad + \quad 21\ O_2(g)$$

$$\downarrow$$

$$6\ N_2(g) + 10\ H_2O\ (g) + 28\ CO_2\ (g) + \text{energy}$$

12,900 kJ
3,225 kJ/mol

Kinetics (speed of reaction) & Gases Produced