Thermochemistry Outline

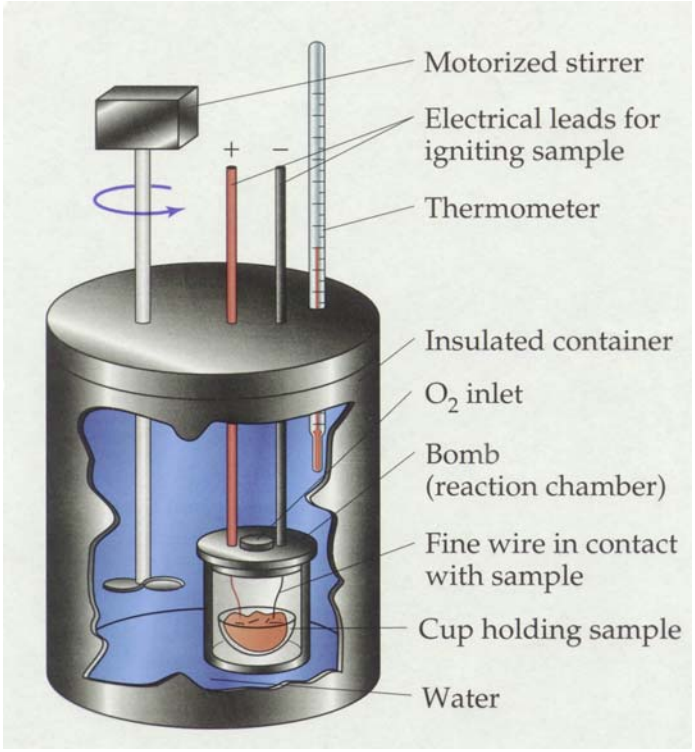
Energy
- Types
  - Potential
  - Kinetic
- Units
  - joules
  - calories
- Total Energy (E_{tot}) = Kinetic Energy (E_k) + Potential Energy (E_p) + U
- Law of Conservation of Energy

Heat (q) vs. Temperature (T)

Heat of reaction
- Exothermic
- Endothermic

Enthalpy
- State Function
- Extensive Property (Review Intensive vs. Extensive properties)
- Enthalpy of Reaction ($\Delta H = \Sigma H_{products} - \Sigma H_{reactants}$)
- Thermochemical Equations

Heat Capacity and Specific Heat
- Measurement of Heat of Reaction
  - Calorimeter



Bomb Calorimeter

The "Bomb" inside is a steel vessel capable of withstanding the large pressure of gas inside as well as the explosive force of the burning reagents inside.

This is a constant volume calorimeter since the reaction occurs within a rigid vessel (the bomb) whose volume cannot change.

The heat capacity of the calorimeter is equal to the sum of the heat capacity of the water + the heat capacity of the dry calorimeter (bomb, stirrer, insulated container, etc):

$C_{calorimeter} = C_{H2O} + C_{dry\ parts}$

If we know $C_{calorimeter}$ and measure ΔT, we can obtain the heat change in the calorimeter.

$\mathbf{q_{calorimeter} = C_{calorimeter} \times \Delta T}$

$\mathbf{\Delta E_{rxn} = q_{rxn} = - q_{calorimeter} = - C_{calorimeter} \times \Delta T}$

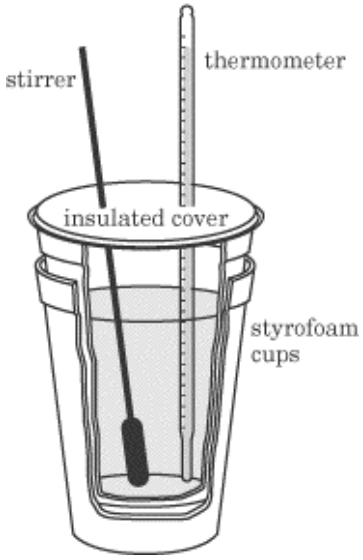
Example: if a reaction performed in a bomb calorimeter is exothermic then the heat absorbed by the calorimeter assembly, $q_{calorimeter}$ is positive (temperature of calorimeter rises)

But this is an exothermic reaction ($\Delta E_{rxn} < 0$) in which no work is done so $q_{rxn} = - q_{calorimeter}$.

In student laboratories the coffee cup calorimeter is typically used.

Hess's Law

Standard Enthalpies of Formation (see attached table)



Operational Skills

- ☐ Calculating kinetic energy.
- ☐ Writing thermochemical equations.
- ☐ Manipulating thermochemical equations.
- ☐ Calculating the heat of reaction from the stoichiometry.
- ☐ Relating heat and specific heat.
- ☐ Calculating ΔH from calorimetric data.
- ☐ Applying Hess's law.
- ☐ Calculating the enthalpy of reaction from standard enthalpies of formation.

Compound	Phase	Formula	ΔH_f° (kJ/mol)
Aluminum			
Aluminum	Solid	Al	0
Aluminum Chloride	Solid	AlCl3	-705.63
Aluminum Oxide	Solid	Al2O3	-1675.7
Barium			
Barium Chloride	Solid	BaCl2	-858.6
Barium Carbonate	Solid	BaCO3	-1213
Barium Oxide	Solid	BaO	-548.1
Barium Sulfate	Solid	BaSO4	-1473.2
Bromine			
Bromine	Liquid	Br2	0
Bromine	Gas	Br	111.884
Bromine	Gas	Br2	30.91
Bromine Trifluoride	Gas	BrF3	-255.6
Hydrobromic Acid	Gas	HBr	-36.29
Calcium			
Calcium	Solid	Ca	0
Calcium	Gas	Ca	178.2
Calcium(II) Ion	Gas	Ca2+	1925.9
Calcium Carbide	Solid	CaC2	-59.8
Calcium Carbonate(Calcite)	Solid	CaCO3	-1207.6
Calcium Chloride	Solid	CaCl2	-795.8
Calcium Phosphate	Solid	Ca3(PO4)2	-4132
Calcium Fluoride	Solid	CaF2	-1219.6
Calcium Hydride	Solid	CaH2	-186.2
Calcium Hydroxide	Solid	Ca(OH)2	-986.09
Calcium Hydroxide	Aqueous	Ca(OH)2	-1002.82
Calcium Oxide	Solid	CaO	-635.09
Calcium Sulfate	Solid	CaSO4	-1434.52
Calcium Sulfide	Solid	CaS	-482.4
Carbon			
Benzene	Liquid	C6H6	48.95
Benzoic acid	Solid	C7H6O2	-385.2
Carbon(Graphite)	Solid	C	0

Compound	Phase	Formula	ΔH_f° (kJ/mol)
Hydrogen			
Hydrogen	Gas	H2	0
Water	Liquid	H2O	-285.83
Water	Gas	H2O	-241.83
Hydrogen Peroxide	Liquid	H2O2	-187.78
Hydrogen Cyanide	Gas	HCN	130.5
Hydrogen Iodide	Gas	HI	26.5
Hydrofluoric Acid	Gas	HF	-269
Hydrochloric acid	Gas	HCl	-92.3
Iodine			
Iodine	Solid	I2	0
Iodine	Gas	I2	62.438
Magnesium			
Magnesium Carbonate	Solid	MgCO3	-1111.69
Magnesium Chloride	Solid	MgCl2	-641.8
Magnesium hydroxide	Solid	Mg(OH)2	-924.54
Magnesium Oxide	Solid	MgO	-601.24
Magnesium sulfate	Solid	MgSO4	-1278.2
Manganese			
Manganese(II) Oxide	Solid	MnO	-384.9
Manganese(IV) Oxide	Solid	MnO2	-519.7
Mercury			
Mercury(II) Oxide (red)	Solid	HgO	-90.83
Mercury Sulfide (red, cinnabar)	Solid	HgS	-58.2
Nitrogen			
Ammonia	Aqueous	NH3	-80.8
Ammonia	Gas	NH3	-45.9
Nitrogen Dioxide	Gas	NO2	33.1
Nitrogen Monoxide	Gas	NO	90.29
Phosphorus			
Phosphorus trichloride	Liquid	PCl3	-320
Phosphorus pentachloride	Solid	PCl5	-440
Potassium			
Potassium Bromide	Solid	KBr	-392.2

Carbon(Diamond)	Solid	C	1.8
Carbon	Gas	C	716.67
Carbon Dioxide	Gas	CO2	-393.509
Carbon disulfide	Liquid	CS2	89.41
Carbon disulfide	Gas	CS2	116.7
Carbon Monoxide	Gas	CO	-110.525
Carbon Tetrachloride	Liquid	CCl4	-139.5
Carbon Tetrachloride	Gas	CCl4	-103.18
Carbonyl Chloride(Phosgene)	Gas	COCl2	-218.8
Ethane	Gas	C2H6	-83.85
Ethanol	Liquid	C2H5OH	-277
Ethanol	Gas	C2H5OH	-235.3
Ethene	Gas	C2H4	52.47
Ethyne	Gas	C2H2	226.73
Methane	Gas	CH4	-74.87
Methanol(Methyl Alcohol)	Liquid	CH3OH	-238.4
Methanol(Methyl Alcohol)	Gas	CH3OH	-201
Methyl Trichloride(Chloroform)	Liquid	CHCl3	-134.47
Methyl Trichloride(Chloroform)	Gas	CHCl3	-103.18
Propane	Liquid	C3H8	-104.7
Chlorine			
Chlorine	Gas	Cl2	0
Chromium			
Chromium	Solid	Cr	0
Copper			
Copper	Solid	Cu	0
Fluorine			
Fluorine	Gas	F2	0

Potassium Chlorate	Solid	KClO3	-397.73
Potassium chloride	Solid	KCl	-436.68
Potassium Fluoride	Solid	KF	-562.6
Silicon			
Silica (Quartz)	Solid	SiO2	-910.86
Silver			
Silver Bromide	Solid	AgBr	-99.5
Silver Chloride	Solid	AgCl	-127.01
Silver Iodide	Solid	AgI	-62.4
Silver Oxide	Solid	Ag2O	-31.1
Silver Sulfide	Solid	Ag2S	-31.8
Sodium			
Sodium Carbonate	Solid	Na2CO3	-1130.77
Sodium Chloride	Aqueous	NaCl	-407.27
Sodium Chloride	Solid	NaCl	-411.12
Sodium Chloride	Liquid	NaCl	-385.92
Sodium Chloride	Gas	NaCl	-181.42
Sodium Fluoride	Solid	NaF	-569
Sodium Hydroxide	Aqueous	NaOH	-469.15
Sodium Hydroxide	Solid	NaOH	-425.93
Sodium Nitrate	Aqueous	NaNO3	-446.2
Sodium Nitrate	Solid	NaNO3	-424.8
Sulfur			
Hydrogen Sulfide	Gas	H2S	-20.63
Sulfur Dioxide	Gas	SO2	-296.84
Sulfuric acid	Liquid	H2SO4	-814