Thermodynamics pre-lab discussion notes and calculations. We will walk you through example lab calculations using nickel (II) nitrate as the salt. You will also be provided data collected in lab for NH_4Cl and $CaCl_2$ to report your results in Canvas.

Videos of procedures:
Procedure video 1 (https://drive.google.com/file/d/1_CoG_V-C-5v_H4SEs8gTD0UEtgmZDZAq/view): ammonium chloride – set up of procedure (measuring salt and water), recording temperature data, and making observation of end of reaction

Procedure video 2 (https://drive.google.com/file/d/1v_BazdJ8XLktKbQ_yTUQ7YcalDBfZ3GR/view): calcium chloride – set up and observation of reaction

We will use nickel (II) nitrate for our calculation examples.
Dissociation or dissolution equation: $Ni(NO_3)_2(s) \rightarrow Ni^{2+}(aq) + 2NO_3^-(aq)$

To calculate the mass of nickel (II) nitrate required to prepare 25 mL of a 2.0 M solution.

$$2.0\ \frac{mol}{L} \times 25\ mL \times \frac{1\ L}{1000\ mL} \times \frac{182.701\ g}{1\ mol} = 9.13505\ g$$

This is the calculation used to determine the mass of each salt that was measured out for this lab.

Example data for nickel (II) nitrate:
Mass of salt: 9.1487 g (our scales measure to 4 decimal places)
Volume of water: 24.8 mL (1 decimal place estimated on 100-mL graduated cylinder)
Initial temperature of water: 22.7°C
Maximum temperature (because temperatures initially increased): 40.8°C

Explanation of temperature data:
In this experiment, the reaction that we are studying is the dissolution (dissolving) of a salt in water. The salt is the reaction and water is the surroundings. Because we are measuring the temperature change of water (the surroundings), when we calculate the heat exchanged, we are calculating qsurr or qsoln. However, we are ultimately interested in determining the heat of reaction (qrxn). Since the reaction takes place in a calorimeter that isolates the heat exchange, any heat released by the reaction is gained by the surroundings and vice versa – any heat gained by the reaction comes from the surroundings. The amount of heat lost by one is equal to the amount of heat gained by the other, they have opposite signs.
Therefore: $\mathbf{q_{soln} = -q_{rxn}}$
Because the calorimeter is not a completely isolated system (there are small air leaks in the lid), temperatures will eventually come back to room temperature. That is why temperature readings are collected for 2 minutes or less.

Example calculations using nickel (II) nitrate to report results
*Note: In the sample calculations below, unrounded values were used to complete each calculation. However, the numbers in parentheses and in RED are rounded to the correct number of significant figure (s.f.) or decimal places (d.p.).

Table 3: Thermodynamic data from textbook:

	ΔH_f^o (kJ/mol)	ΔG_f^o (kJ/mol)	S^o (J/K·mol)	
$Ni(NO_3)_2$	-415.0	-222.2	192.0	Data used in pre-lab example calculations
Ni^{2+}(aq)	-64.0	-46.4	-159.0	
NO_3^-	-205.0	-108.7	146.4	
NH_4Cl (s)	-314.43	-202.87	94.6	Data to be used in Canvas questions
NH_4^+ (aq)	-132.5	-79.31	113.4	
Cl^- (aq)	-167.2	-131.2	56.5	
$CaCl_2$ (s)	-795.8	-748.1	104.6	
Ca^{2+} (aq)	-542.96	-553.04	-55.2	

Sample calculations:

1) Moles of salt: use measured mass of salt and molar mass to calculate moles

$$\text{moles} = 9.1487\ g \times \frac{1\ mol}{182.701} = 0.050075\ mol$$

2) Mass of water: use density of water (1.00 g/mL) to convert measured volume to grams

$$\text{mass of water} = 24.8\ mL \times \frac{1.00\ g}{1\ mL} = 24.8\ g$$

3) Mass of solution: add the measured mass of salt and calculated mass of water

mass of solution = 9.1487 g + 24.8 g = 33.9487 g (33.9 g: addition – least decimal places)

4) Final temperature (**maximum** temperature): 40.8°C

5) ΔT (°C) = $T_f - T_i$ (T_i is the **initial temperature** before the salt and water are combined) = 40.8°C – 22.7°C = 18.1°C

6) $q_{rxn} = -\ q_{soln}$

q_{soln} = mass solution x specific heat of water x ΔT

q_{soln} = 33.9487 g x 4.184 J/g·°C x 18.1°C = 2570.9 J (2570 J: multiplication – least sig. figs)

$q_{rxn} = -q_{soln}$ = -2570.9 J (-2570 J)

7) Enthalpy of reaction:

$$\Delta H_{rxn} = \frac{q_{rxn}}{moles\ of\ salt} = \frac{-2570.9\ J}{0.0050075\ moles} = -51340\ \frac{J}{mol} \times \frac{1\ kJ}{1000\ J}$$

$$= -51.340\frac{kJ}{mol}\left(-51.3\frac{\text{kJ}}{\text{mol}}\ \text{: multiplication - least sig. figs}\right)$$

8) Entropy of reaction using standard thermodynamic data from Table 3 on the previous page:

$\Delta S^o_{rxn} = \Sigma n\ S^o_{\text{(products)}} - \Sigma n\ S^o_{\text{(reactants)}}$

ΔS^o_{rxn} = [1 mol Ni^{2+}(-159.0 J/Kmol) + 2 mol NO_3^-(146.4 J/K mol)] –
[1 mol $Ni(NO_3)_2$(192.0 J/K mol)] = -58.2 J/K (subtraction: least decimal places)

9) Free Energy of reaction: In this calculation, T is the **initial temperature** (before the salt and water are combined).

$\Delta G_{rxn} = \Delta H_{rxn} - T \times \Delta S^o_{rxn}$

ΔG_{rxn} = -51.3 kJ/mol – ((273.15 + 22.7)K x -0.0582 kJ/K) ← note units of ΔH vs ΔS!

ΔG_{rxn} = -34.1 kJ (report answer to 1 decimal place (like in ΔH and ΔS))

Thermodynamics Lab Data

Data and Calculations

Table 1: Masses of salts, volume of water, initial temperature, and temperature of dissolution

	Ammonium Chloride		**Calcium Chloride**
Mass of salt, g	**2.6671**	Mass of salt, g	**5.5721**
Volume of water, mL	**24.5**	Volume of water, mL	**25.1**
Initial temperature, T_i (°C)	**20.8**	Initial temperature, T_i (°C)	**20.9**
Time	**Temperature, °C, Trial 1**	**Time**	**Temperature, °C, Trial 1**
0:00	19.6	0:00	21.5
0:10	13.5	0:10	39.8
0:20	12.9	0:20	48.4
0:30	***12.8 (min.**	0:30	49.4
0:40	12.9	0:40	53.6
0:50	12.9	0:50	53.7
1:00	12.9	1:00	***56.2 (max.**
1:10	12.9	1:10	54.2
1:20	13.0	1:20	53.9
1:30	Temperature data	1:30	53.5
1:40		1:40	53.1
1:50		1:50	52.7
2:00		2:00	52.4

You will be asked to complete the following calculations for each salt:

1) moles of salt
2) mass of water
3) mass of solution
4) final temperature
5) ΔT
6) q_{soln} and q_{rxn} (J)
7) ΔH_{rxn} (kJ/mol)
8) ΔS^{o}_{rxn} (J/K)
9) ΔG_{rxn} (kJ/mol)