

# cheg325 hw2q2 coding for tedious math

AUTHOR  
k.wodehouse

PUBLISHED  
February 16, 2025

These calculations are extremely easy, but doing them by hand is prone to errors. i put the data in a tab-separated text file and imported it here as a pandas dataframe to lower the chances of human errors.

```
import numpy as np
import pandas as pd
df = pd.read_csv('a3.txt', sep='\t', index_col=0)
df
```

	h_formation	g_formation
species		
N2	0.0	0.0
H2	0.0	0.0
NH3	-46.1	-16.5
C3H8	-104.7	-24.3
C2H4	52.5	68.5
CH4	-74.5	-50.5
CaCO3	-1206.9	-1128.8
CaO	-635.1	-604.0
CO2	-393.5	-394.4
CO	-110.5	-137.2
H2O	-241.8	-228.6

(a)

```
species = ['N2', 'H2', 'NH3']
coeffs = np.array([-1,-3,2])

new_df = df.loc[species]
H_form = (new_df['h_formation'] * coeffs).sum()
G_form = (new_df['g_formation'] * coeffs).sum()
print(f'ΔH rxn: {H_form:.1f} kJ/mol')
print(f'ΔG rxn: {G_form:.1f} kJ/mol')
```

ΔH rxn: -92.2 kJ/mol  
ΔG rxn: -33.0 kJ/mol

(b)

```
species = ['C3H8', 'C2H4', 'CH4']
coeffs = np.array([-1, 1, 1])

new_df = df.loc[species]
H_form = (new_df['h_formation'] * coeffs).sum()
G_form = (new_df['g_formation'] * coeffs).sum()
print(f'ΔH rxn: {H_form:.1f} kJ/mol')
print(f'ΔG rxn: {G_form:.1f} kJ/mol')
```

ΔH rxn: 82.7 kJ/mol  
ΔG rxn: 42.3 kJ/mol

(c)

```
species = ['CaCO3', 'CaO', 'CO2']
coeffs = np.array([-1, 1, 1])

new_df = df.loc[species]
H_form = (new_df['h_formation'] * coeffs).sum()
G_form = (new_df['g_formation'] * coeffs).sum()
print(f'ΔH rxn: {H_form:.1f} kJ/mol')
print(f'ΔG rxn: {G_form:.1f} kJ/mol')
```

ΔH rxn: 178.3 kJ/mol  
ΔG rxn: 130.4 kJ/mol

(d)

```
species = ['CO', 'H2', 'CH4', 'CO2', 'H2O']
coeffs = np.array([-4, -8, 3, 1, 2])

new_df = df.loc[species]
H_form = (new_df['h_formation'] * coeffs).sum()
G_form = (new_df['g_formation'] * coeffs).sum()
print(f'ΔH rxn: {H_form:.1f} kJ/mol')
print(f'ΔG rxn: {G_form:.1f} kJ/mol')
```

ΔH rxn: -658.6 kJ/mol  
ΔG rxn: -454.3 kJ/mol

```
# this is filler text.
```