Mahler Bomb

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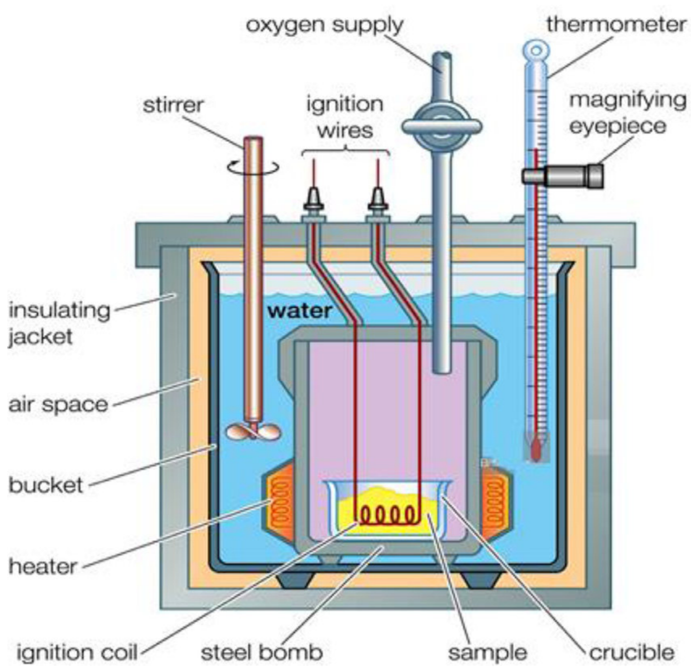
1 Bomb Description

Mahler Bomb is a calorimeter to measure the internal energy of a substance.
The system comprises 3 concentric cylinders: the innermost contains the substance that we want to measure the internal energy, between the first and second one there is distilled water ($V_{H_2o} = 2.2l$), and the outermost is an adiabatic cylinder to isolate the system from the outside. A mixer avoids temperature gradients inside the water when the bomb explodes and a pt100 is used to measure the temperature inside the water.
Oxygen is put inside the bomb in stoichiometric excess in such a way as to favour the chemical reaction. In order to do that we dilute the air inside the bomb 3 times with oxygen and then we pump oxygen at 18 bar.



2 Calibration

Firstly we want to find the specific heat capacity of the entire system, in order to do that we use benzoic acid.
The chemical reaction that occurs is:

$$C_7H_6O_2(s) + \frac{15}{2}O_2(g) \rightarrow 7CO_2(g) + 3H_2O(l) \tag{1}$$

We know that:

$$H = U + PV \tag{2}$$

Differentiating:

$$\Delta H = \Delta U + \Delta(PV) \tag{3}$$

We approximate that the term $\Delta(PV)$ is only due to the gas because it expands much more compared to the solid and liquid phases, so we can use the perfect gas equation: $PV = nRT$:

$$\Delta H = \Delta U + \Delta(nRT) \tag{4}$$

so:

$$\Delta H = \Delta U + \Delta(n)R\bar{T} + \bar{n}R\Delta(T) \tag{5}$$

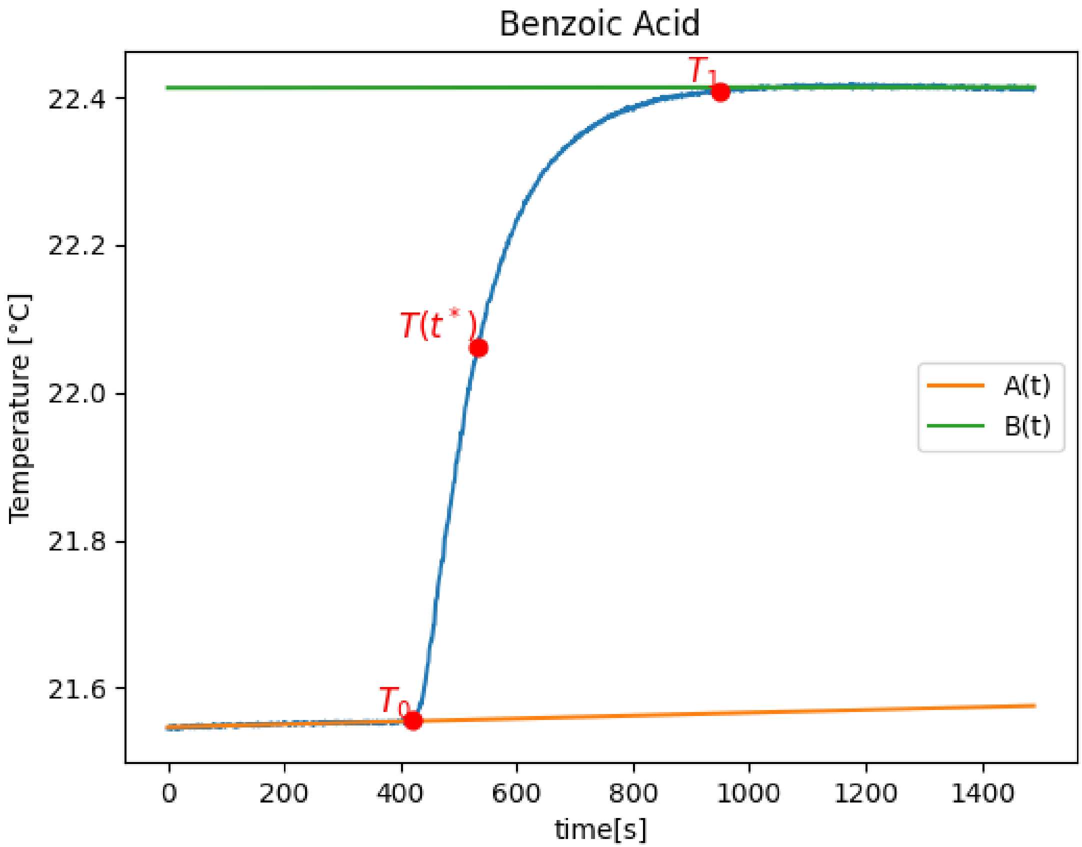
Where $\bar{T}$ and $\bar{n}$ are the mean values of temperature and moles before and after the chemical reaction.
The temperature variation is very small $\Delta T \approx 0$ so the last term can be neglected:

$$\Delta H = \Delta U + \Delta(n)R\bar{T} \tag{6}$$

So:

$$\Delta U = \Delta H - \Delta(n)R\bar{T} \tag{7}$$

To find the variation of temperature ΔT we find the two lines through linear regression before($A(t)$) and after the bomb explosion($B(t)$) . Then we find the point of temperature before the explosion when the line changes the gradient(T_0) and the point of temperature after the explosion when the exponential rise of temperature comes back to a line(T_1).
We calculate $60\% \cdot (T_1 - T_0)$ and the time t^* that corresponds to $T(t^*) = T(0) + 60\% \cdot (T_1 - T_0)$.
Finally, we find the variation of temperature as $\Delta T = B(t^*) - A(t^*)$.
This procedure is done to reduce the temperature noise.



Exploiting this procedure we find that $\Delta T_{benz} = 0.86 \pm 0.04K$.
We find $\Delta n_{benz} = \frac{15}{2} - 7 = -0.5$, $\bar{T}_{benz} = 295.1 \pm 0.8K$ and R is gas constant: $R = 8.314\frac{J}{molK}$.
The mass of benzoic acid is $m_{ben} = 0.41 \pm 0.02g$, the molar mass is $m_{mol_{ben}} = 122.12g/mol$ so the number of moles that react are: $n_{ben} = \frac{m_{benz}}{m_{mol_{ben}}} = 3.0 \pm 0.2mmol$.
We know that the nominal value of the enthalpy variation of combustion per mole of benzoic acid is $\Delta H = -3227KJ/mol$ so we can find using [7] $\Delta U_{benz} = -3.23 \pm 12MJ/mol$. To find the energy released in the combustion: $\Delta U_{comb} = n_{ben}\Delta U_{benz} = 10.8 \pm 0.4KJ$
So now we can find c_v:

$$c_v = \frac{\Delta U_{comb}}{\Delta T_{ben}} = 12.7 \pm 0.6\frac{KJ}{K} \tag{8}$$

3 Isooctane

Now that we have found c_v of the system we can easily find ΔU:

$$\Delta U = \frac{c_v \Delta T}{n} \tag{9}$$

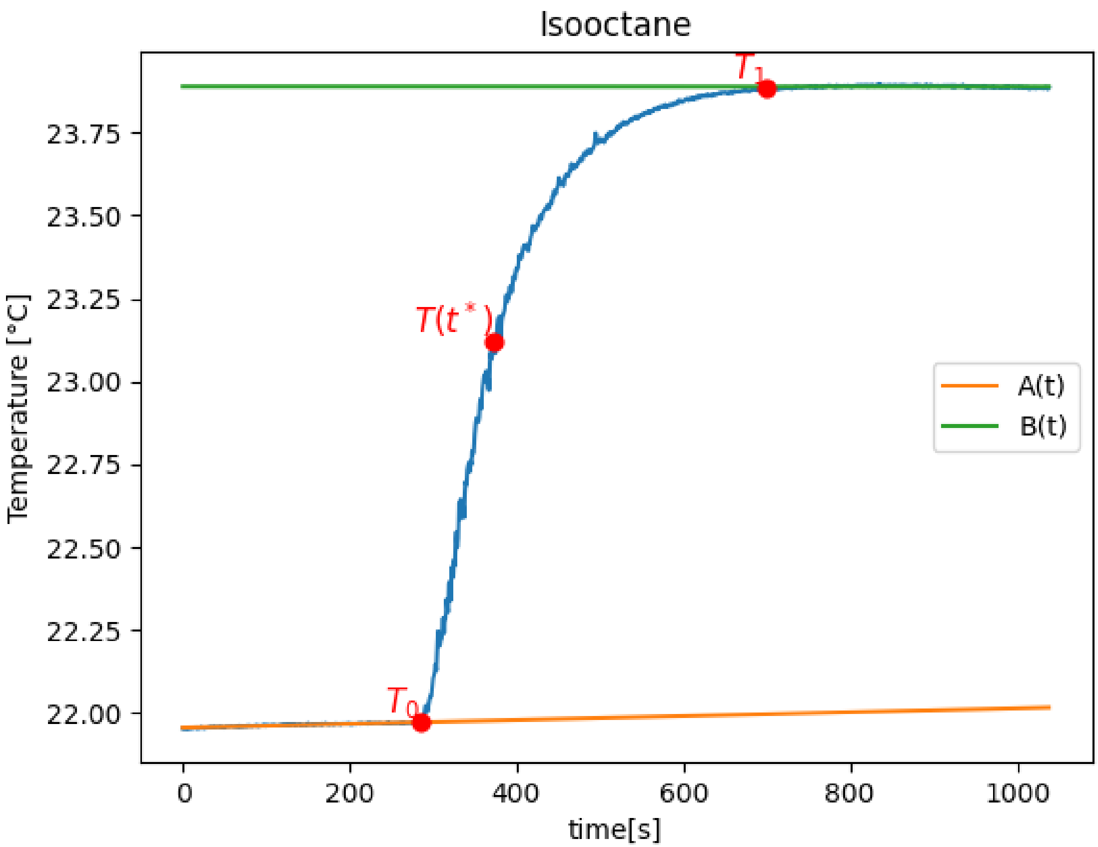
So:

$$\Delta H = \Delta U + \Delta(n)R\bar{T} \tag{10}$$

The chemical reaction that occurs is:

$$C_8H_{18}(l) + \frac{25}{2}O_2(g) \rightarrow 8CO_2(g) + 9H_2O(l) \tag{11}$$

The volume of isooctane is $V_{iso} = 0.7 \pm 0.1 \cdot 10^{-6}m^3$, the density $\rho_{iso} = 690kg/m^3$ so the mass: $m_{iso} = \rho_{iso} \cdot V_{iso} = 0.48 \pm 0.02g$, $\Delta(n) = -4.5$. The molar mass is $m_{mol_{iso}} = 114.23g/mol$, so $n_{iso} = \frac{m_{iso}}{m_{mol_{iso}}} = 4.2 \pm 0.2mmol$.
We find that $\Delta T_{iso} = 1.9 \pm 0.1K$, $\bar{T}_{iso} = 296.1 \pm 0.9K$ so we can calculate $\Delta H_{iso} = \frac{c_v \cdot \Delta T_{iso}}{n_{iso}} + \Delta(n)R\bar{T}_{iso} = -5.74 \pm 0.24\frac{MJ}{mol}$.

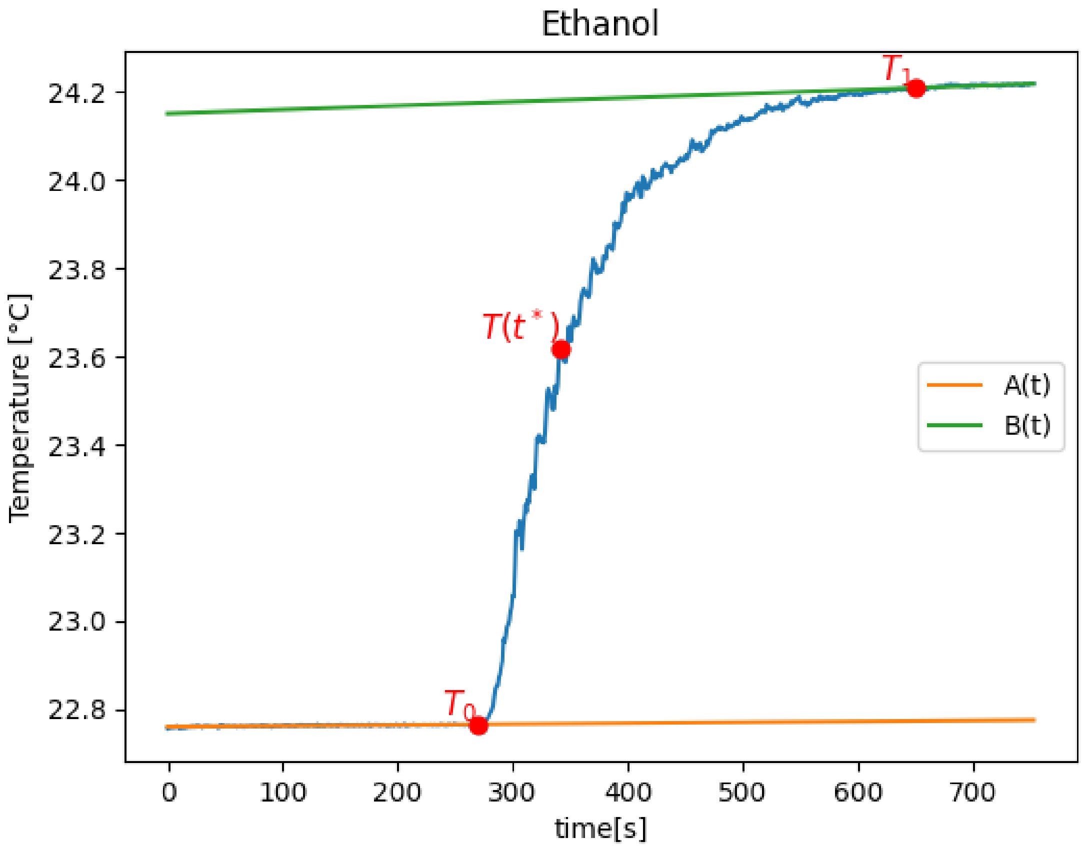


4 Ethanol

The chemical reaction that occurs is:

$$C_2H_6O(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(l) \tag{12}$$

The volume of ethanol is $V_{et} = 0.8 \pm 0.1 \cdot 10^{-6} m^3$, the density $\rho_{et} = 789 kg/m^3$ so the mass: $m_{et} = \rho_{et} \cdot V_{et} = 0.63 \pm 0.02 g$, $\Delta(n) = -1$. The molar mass is $m_{mol_{et}} = 46.068 g/mol$, so $n_{et} = \frac{m_{et}}{m_{mol_{et}}} = 13.7 \pm 0.6 mmol$.
We find that $\Delta T_{et} = 1.4K \pm 0.1$ and $\bar{T}_{et} = 296.7 \pm 0.4K$ so we can calculate $\Delta H_{et} = c_v \cdot \Delta T_{et} + \Delta(n) R \bar{T}_{et} = -1.31 \pm 0.06 \frac{MJ}{mol}$



5 Summary

	n moli[mmol]	mass[g]	$\Delta H[\frac{MJ}{mol}]$
Benzoic acid	3.0 ± 0.2	0.41 ± 0.01	-3.227
Isooctane	4.2 ± 0.2	0.48 ± 0.02	-5.74 ± 0.24
Ethanol	13.7 ± 0.6	0.63 ± 0.02	-1.31 ± 0.06

We find that $c_v = 12.7 \pm 0.6 \frac{KJ}{K}$.