

Therm – Thermodynamic Quantities by Linear System at Two Temperatures

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This program is intentionally simple, yet it allows the simultaneous calculation of ΔS and ΔH by linear algebra for a pair of reactions occurring at different temperatures, given known values of ΔG (*linear system of equations*). It was developed using the [newRPL firmware](#), although it can be easily adapted to the original HP50G firmware.

1 Equation:

$$\Delta G^{T_1} = \Delta H - T_1 \cdot \Delta S$$

$$\Delta G^{T_2} = \Delta H - T_2 \cdot \Delta S$$

The solution is obtained via matrix algebra:

$$A \cdot x = b$$

Where:

- A = matrix containing temperature values and a unitary first column;
- b = column matrix with ΔG values
- x = resulting matrix containing the parameters ΔS and ΔH .

2 Files:

1. Program
2. Source code

3 Usage:

To run the program, the following data must be entered sequentially on the stack:

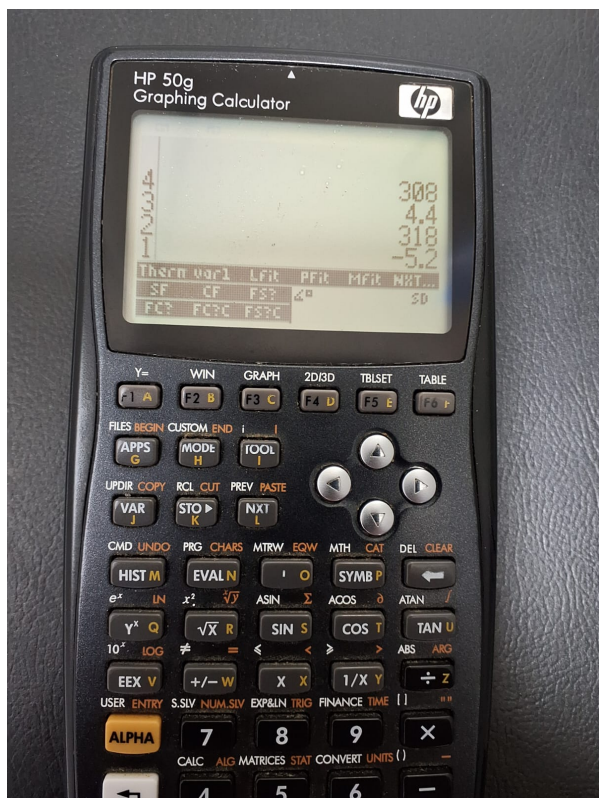
```
# Data input
```

```
1. DeltaG_1, T1, DeltaG_2, T2;
```

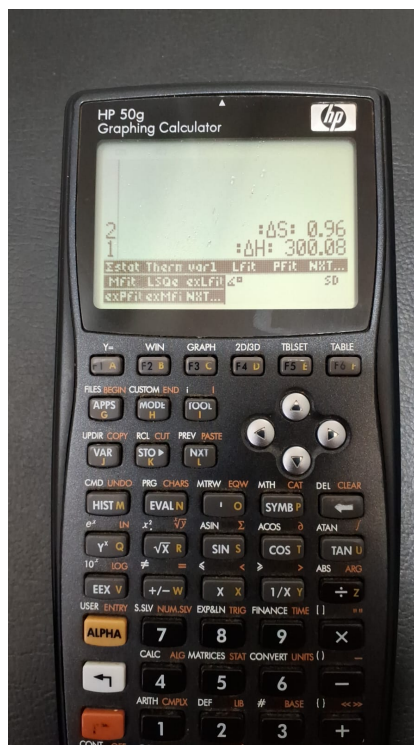
```
2. After selecting "Therm", the program computes the values of DeltaS and DeltaH.
```

4 Example

The figure below illustrates the HP50G with data input and the resulting stack output for the reaction described in Cooper (2011), as well as the *newRPL* firmware layout.



(a) Input of ΔG and T_1 , and ΔG and T_2 values.



(b) Results obtained from the program.

Figure 1: Execution of the *Therm* program to obtain ΔS and ΔH for a chemical reaction at two temperatures (*newRPL* firmware). The results are consistent with those reported by the author (Cooper, 2011).

References

1. Cooper, Alan. *Biophysical Chemistry*. Royal Society of Chemistry, No. 24, p. 113, 2011.

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