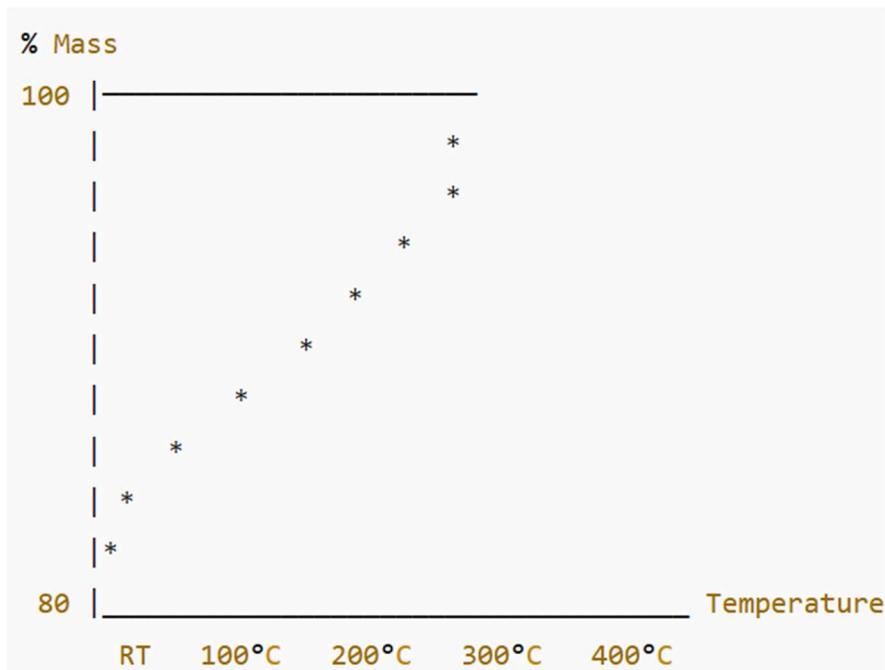# TGA (Thermogravimetric Analysis) graph of CaSO₄ (calcium sulfate)

For **CaSO₄ and its hydrates**, what's important is the loss of water molecules from the crystal structure as temperature increases.

TGA curve for CaSO₄·2H₂O:

```
% Mass
100 |——————————————————
    |
    |                        *
    |                        *
    |                     *
    |                  *
    |              *
    |           *
    |        *
    |     *
    |   *
    | *
 80 |_____ Temperature
      RT    100°C    200°C    300°C    400°C
```

What Happens to Calcium Sulfate (CaSO₄) in TGA?

Calcium sulfate exists in different hydration forms:

- **Gypsum (CaSO₄·2H₂O)** has 2 molecules of water.
- **Hemihydrate (CaSO₄·0.5H₂O)** has half a molecule.
- **Anhydrite (CaSO₄)** is the dry, anhydrous form

The overall dehydration process can be represented as:

1. **CaSO₄·2H₂O → CaSO₄·0.5H₂O + 1.5 H₂O** (first dehydration)
2. **CaSO₄·0.5H₂O → CaSO₄ + 0.5 H₂O** (complete dehydration)

Typical Steps on a TGA Graph

When heating **CaSO₄·2H₂O (gypsum)**:

1. **Initial Plateau**
   From room temperature up to ~100–150 °C, the weight stays almost constant (removes adsorbed surface water).

2. **First Major Weight Loss (Dehydration)**
Around ~150–300 °C the sample loses structural water — converting from **gypsum to hemihydrate and then to anhydrite**. This shows up as a **steep drop in the TGA curve**, typically amounting to about **21% weight loss** (for full dehydration from $CaSO_4 \cdot 2H_2O$ to $CaSO_4$).
3. **Plateau After Dehydration**
After about ~300–400 °C, once all water is gone, the mass becomes stable (no further weight loss).
4. **(At very high T > 1200 °C)**
Further thermal breakdown of $CaSO_4$ may occur, losing SO_3, but most basic TGA studies stop before that.

Step 1: Molar Masses

We need the molar masses of hydrated and dehydrated forms:

- **CaSO₄·2H₂O (gypsum)**
  Ca = 40.08, S = 32.07, O₄ = 4×16 = 64, 2H₂O = 2×18.02 = 36.04
  → **Total ≈ 172.17 g/mol**
- **CaSO₄·0.5H₂O (hemihydrate)**
  CaSO₄ = 136.15, 0.5H₂O = 0.5×18.02 = 9.01
  → **≈ 145.16 g/mol**
- **CaSO₄ (anhydrite)**
  Ca = 40.08, S = 32.07, O₄ = 64
  → **≈ 136.15 g/mol**

Step 2: Weight Loss on First Dehydration

This is the loss of **1.5 H₂O** when gypsum becomes hemihydrate.

- Water lost = 1.5 × 18.02 = **27.03 g**
- Percentage loss:

$$\text{Residue: } \frac{23.07}{172.17} \times 100 \approx 15.7\%$$

So around **15.7% mass loss** is seen on the TGA during the first step.

Step 3: Weight Loss on Final Dehydration

Hemihydrate → Anhydrite releases **0.5 H₂O**:

- Water lost = 0.5 × 18.02 = **9.01 g**
- Percentage loss (relative to original gypsum):

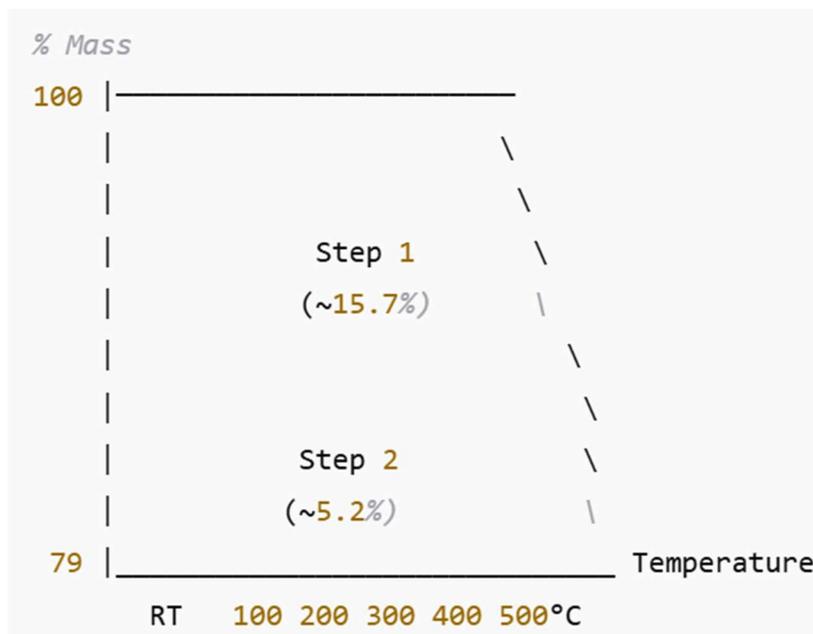$$\text{Residue: } \frac{9.01}{172.17} \times 100 \approx 5.23\%$$

So this step contributes about **5.2% mass loss**.

Total Weight Loss

Sum of both:

- **15.7% + 5.2% ≈ 20.9%**

This is the **expected total mass loss** when $CaSO_4 \cdot 2H_2O$ fully dehydrates to $CaSO_4$.

```
% Mass
100 |————————————————————
    |                      \
    |                       \
    |          Step 1        \
    |          (~15.7%)        \
    |                           \
    |                            \
    |          Step 2             \
    |          (~5.2%)             \
 79 |_____  Temperature
      RT   100 200 300 400 500°C
```

- **Plateau at ~100–150 °C:** small bound water may be removed.

- **First steep drop (~150–250 °C):** ~15.7% loss (dihydrate → hemihydrate).

- **Second drop (~250–350 °C):** ~5.2% loss (hemihydrate → anhydrite).

- **Above ~400 °C:** mostly stable $CaSO_4$, no further water loss unless decomposition happens at very high T.

Interpretation

1. **The shape of the TGA curve reflects dehydration stages.**
   Each drop corresponds to water leaving the structure at specific temperature ranges.
2. **Calculated mass losses match theory.**
   The total ~20.9% loss agrees with the stoichiometry of water content (2 H_2O per formula unit).

3. **Quantitative TGA is useful to identify hydrates.**
   By comparing measured mass loss with calculated values, you can tell whether the sample is dihydrate, hemihydrate, or anhydrite.