

Back Isomerization Kinetics of Molecular Photoswitches : Complementary Insights from Liquid Chromatography and Ion Mobility Measurements

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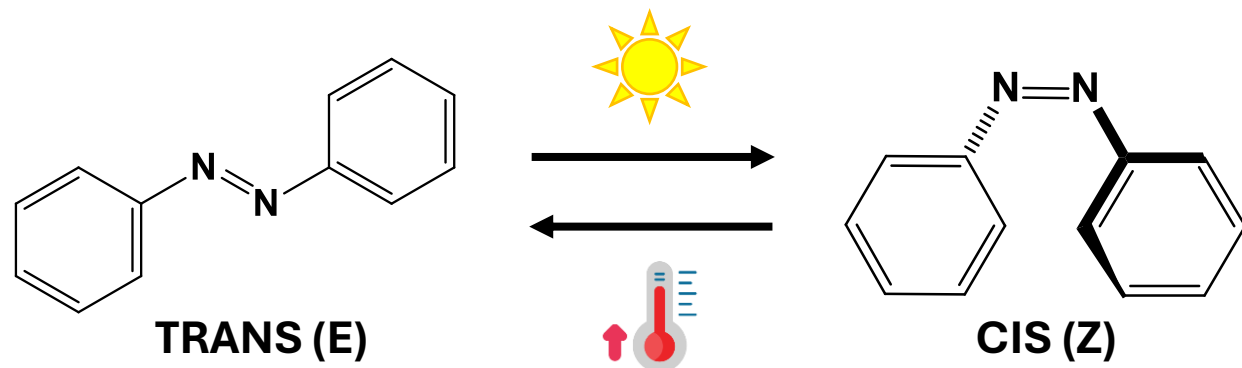
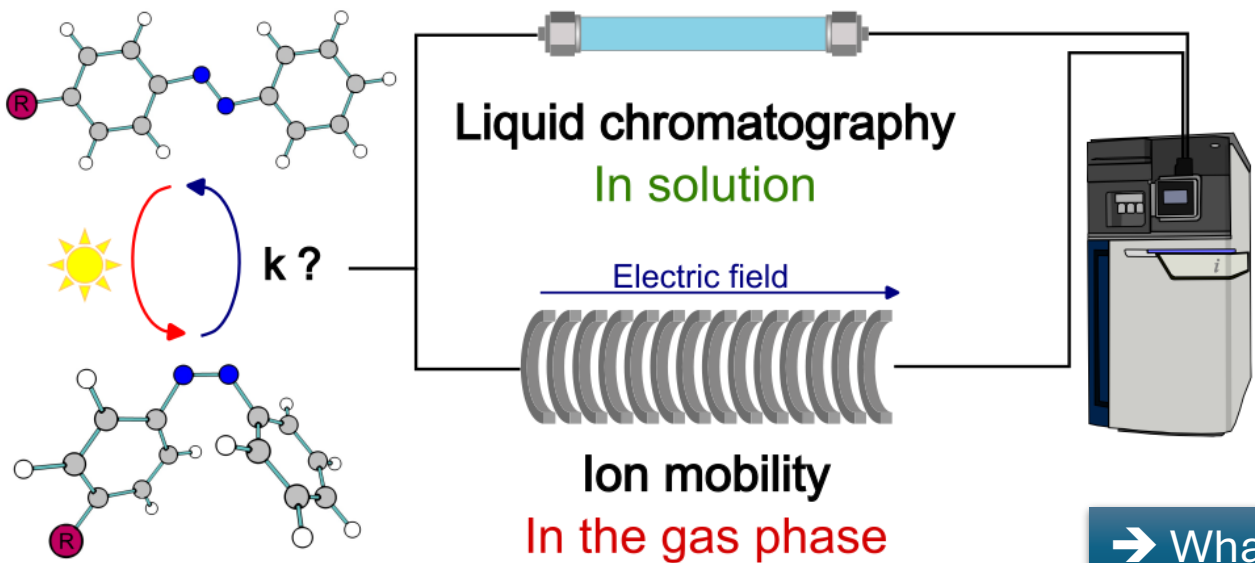


How to store solar energy ?



- Solar energy storage is essential
- Storage using organic photoswitches → *MOST*

MOST - Molecular Solar Thermal Energy Storage Systems



Thermal back-isomerization process ???

In **solution**:

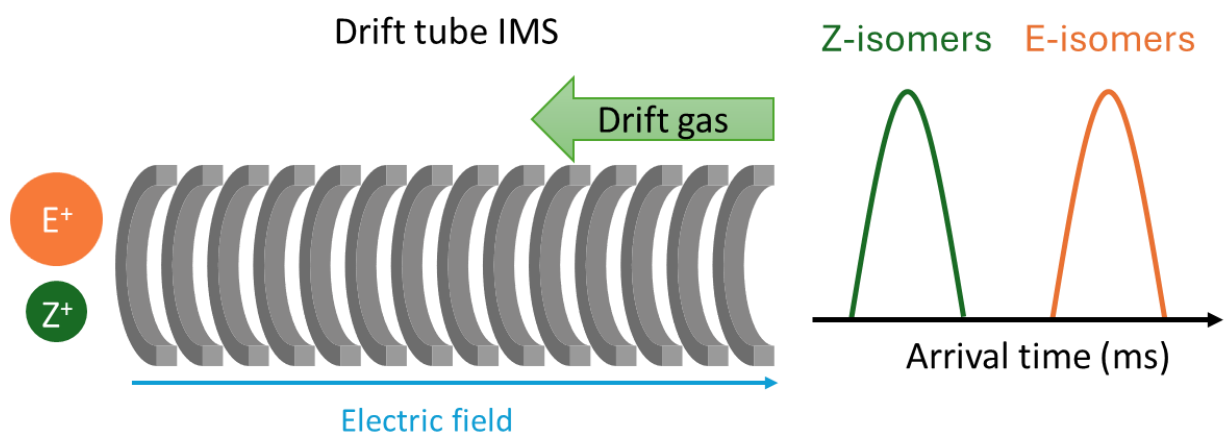
- Solvent dependence
- Photoisomer separation
- Time and temperature limitations

Studying thermal isomerization process is very complex...

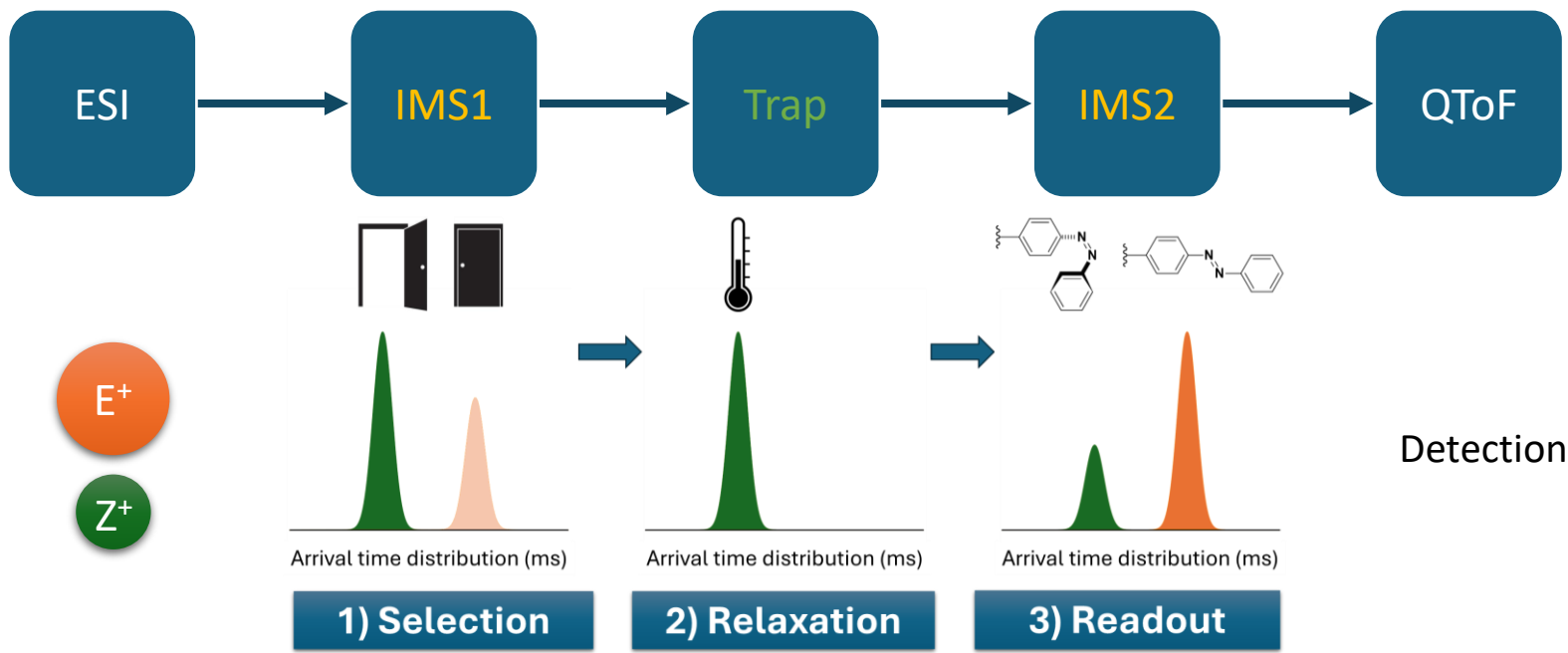
➔ What about measuring thermal isomerization in the **gas phase** ?

... and here comes the home-built tandem IMS device

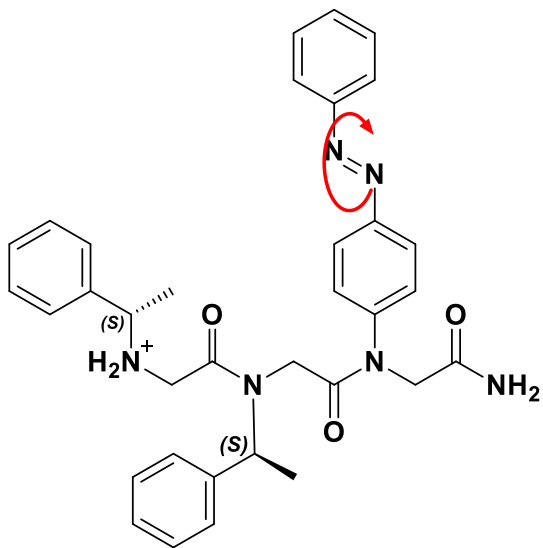
- 1) Z-photoisomers selection in **IMS1**
- 2) Trapped ion relaxation at a controlled temperature for a variable time
= **kinetic monitoring** (different T)
- 3) Photoisomer population sampling by **IMS2**



Photoisomer ion separation based on their **collisional cross section CCS**



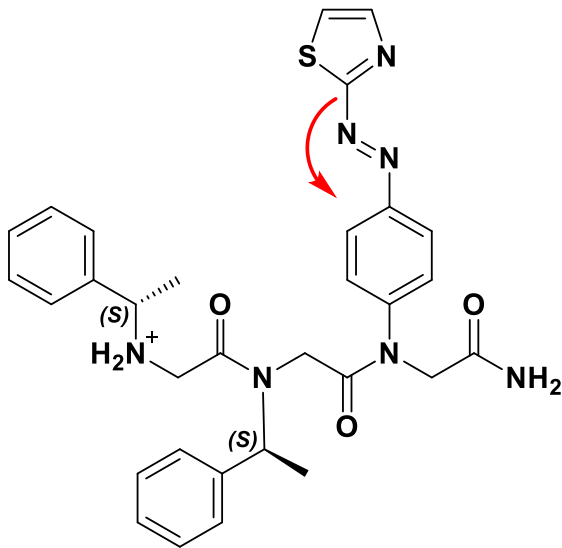
What can you obtain from back-isomerization kinetics ?



$$\Delta H^\ddagger = 101.64 \pm 1.83 \text{ kJ mol}^{-1}$$

$$\Delta S^\ddagger = -25.42 \pm 0.53 \text{ J mol}^{-1} \text{ K}^{-1}$$

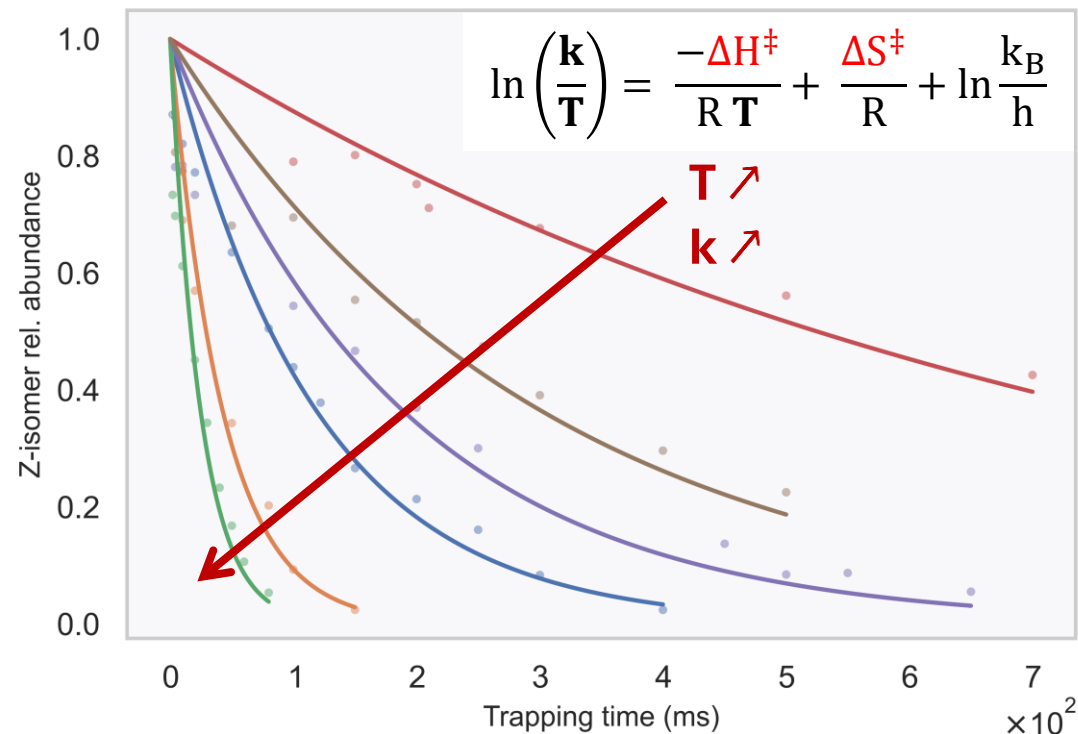
Back-isomerization by
rotation



$$\Delta H^\ddagger = 93.08 \pm 0.48 \text{ kJ mol}^{-1}$$

$$\Delta S^\ddagger = 9.85 \pm 0.05 \text{ J mol}^{-1} \text{ K}^{-1}$$

Back-isomerization by
inversion



- Thermal back-isomerization mechanism elucidation
- Correlation between solution and gas-phase

**analytical
chemistry**



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Thank you for your attention!



A good point of view



Fête des Lumières



And the lab...

