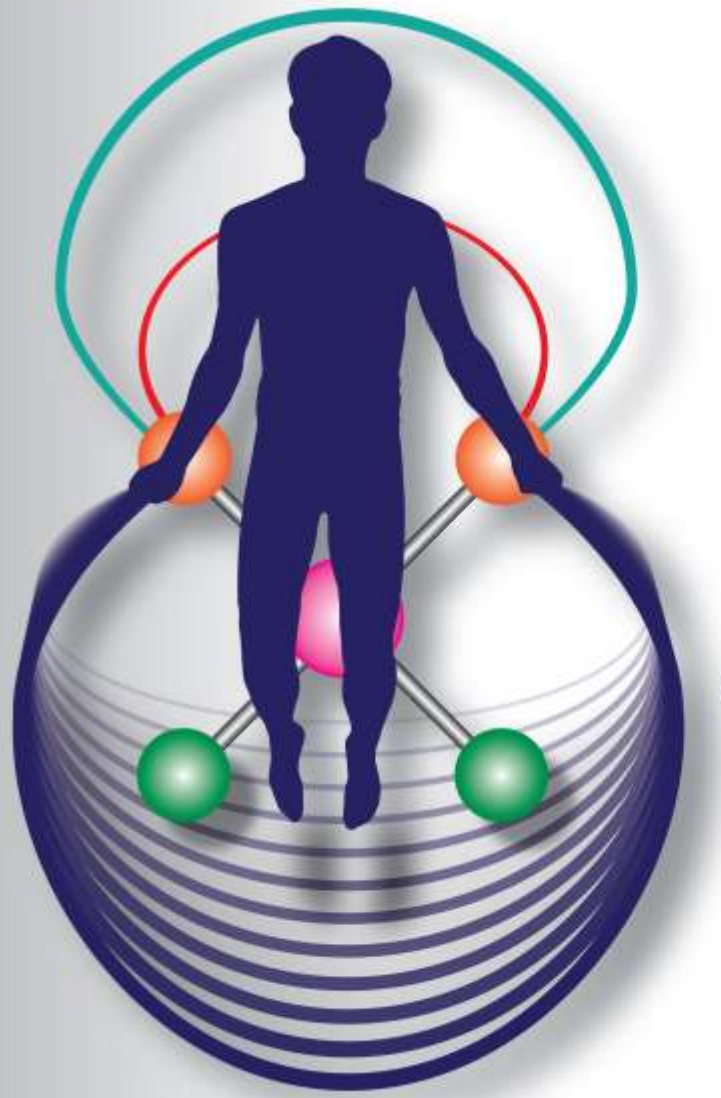
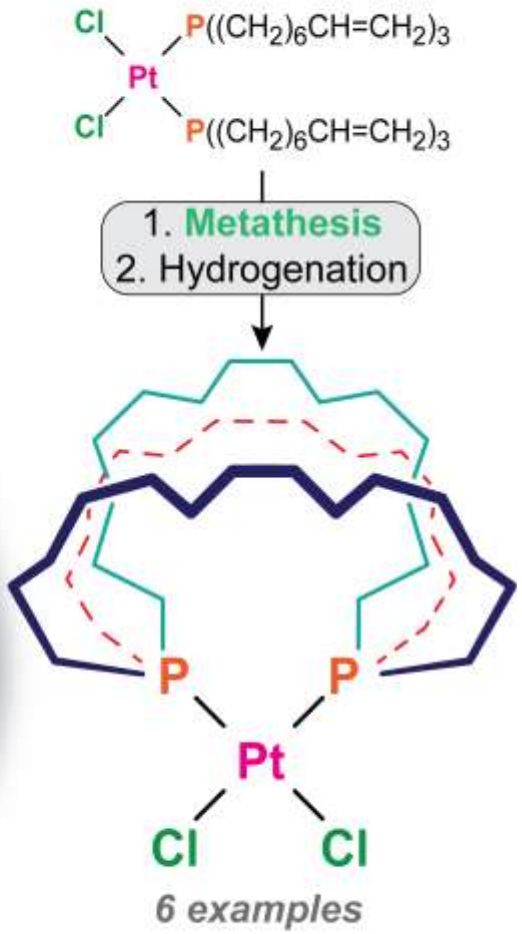
HPRC SC 2019





MOLECULAR JUMP-ROPE: MULTIRINGED METAL-COMPLEXES THAT REALLY KNOW HOW TO JUMP

"The platinum complexes described can undergo a "triple jump rope" mechanism rendering the three methylene chains of their ligands equivalent, a motion that is unheard of and reminiscent of Olympic traditions such as the triple-Axel or the triple jump."

— Dr. John Gladysz

TAMU CHEMISTRY

Joshi, H.; Kharel, S.; **Ehnbom, A.**; Skopek, Hess, G. D.; Fiedler, T.; Hampel, F.; Bhuvanesh, N.; Gladysz, J. A. *J. Am. Chem. Soc.* **2018**, *140*, 8463

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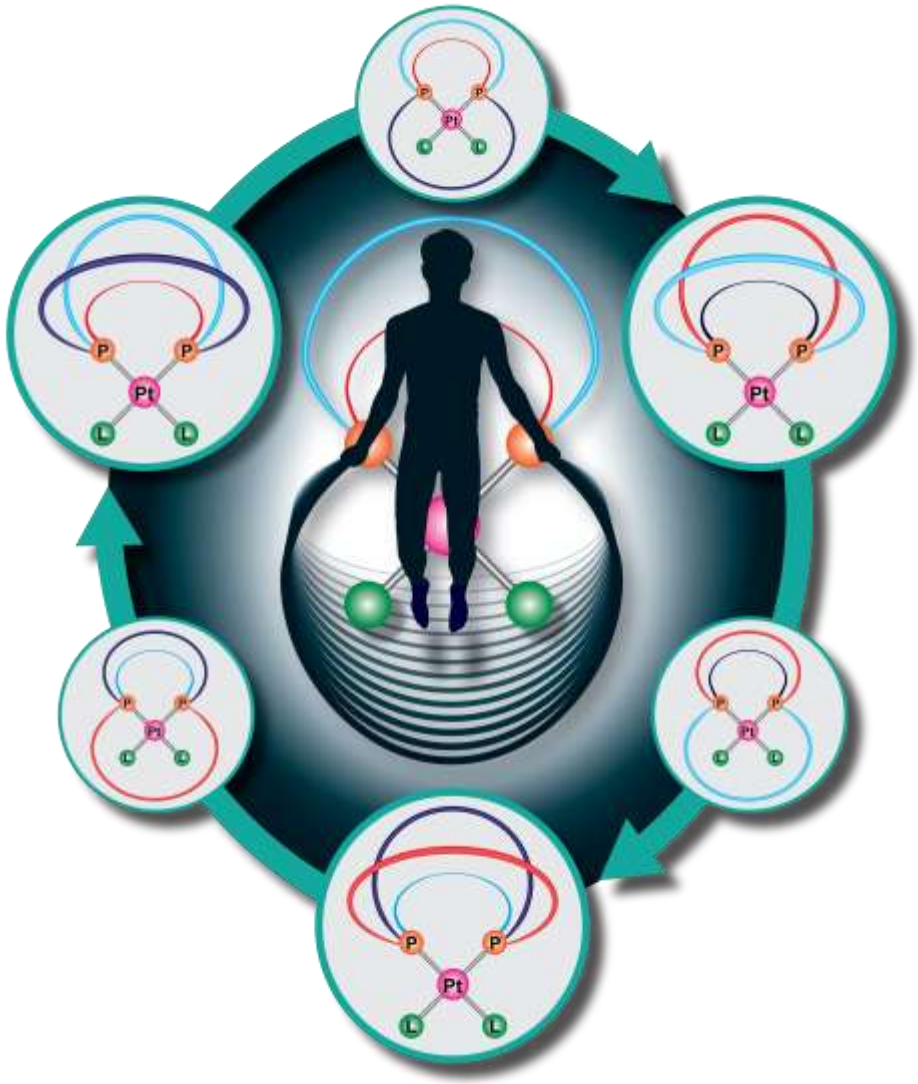

INTRODUCTION

- Molecular devices mimicking the properties of a ***molecular rotor*** where featuring a rotating and a static component is sought.
- Novel "jump-rope" process was observed in these "***parachute*** ***complexes*** while attempting to make ***molecular gyroscopes*** with a different design.
- One potential application of these is the miniaturization of electronic components.

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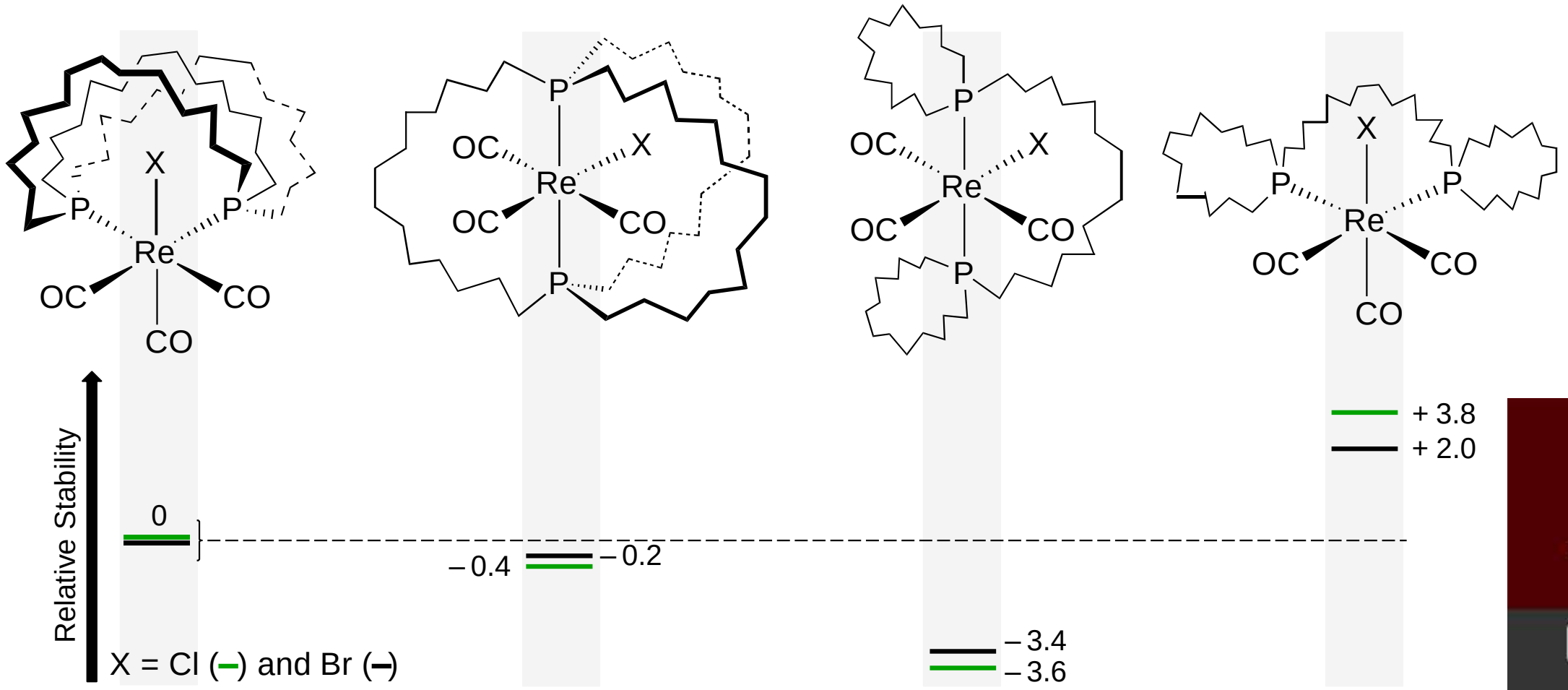
SELECTED DATA

- Computing relative thermodynamic stability of byproducts in ***molecular devices***



CHEMISTRY

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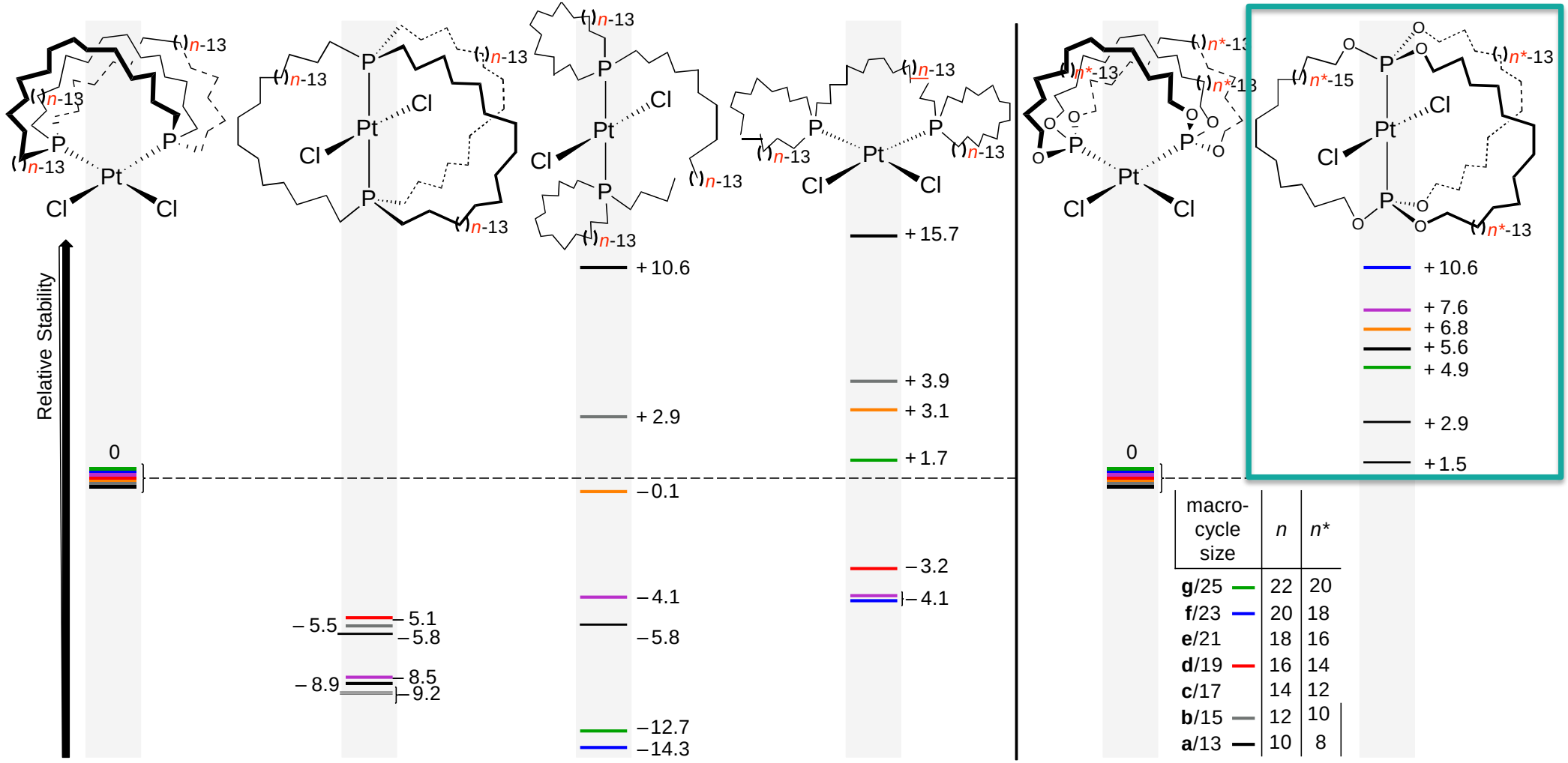
- Predicting reaction outcome before performing experiments.



not observed in experiments

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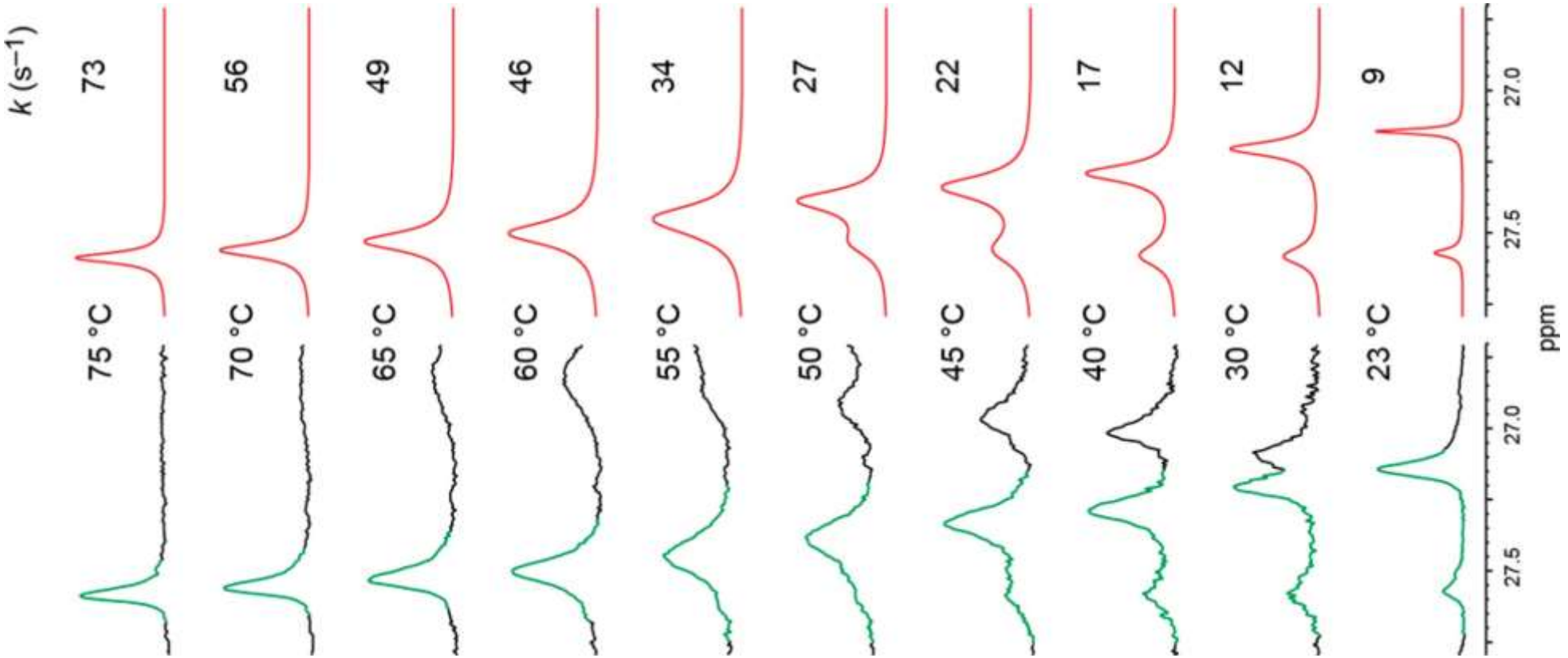
SELECTED DATA

- **Simulated** spectroscopic data at different temperature to obtain ***rotational barriers***.



- **Experimental** spectroscopic data at different temperatures.

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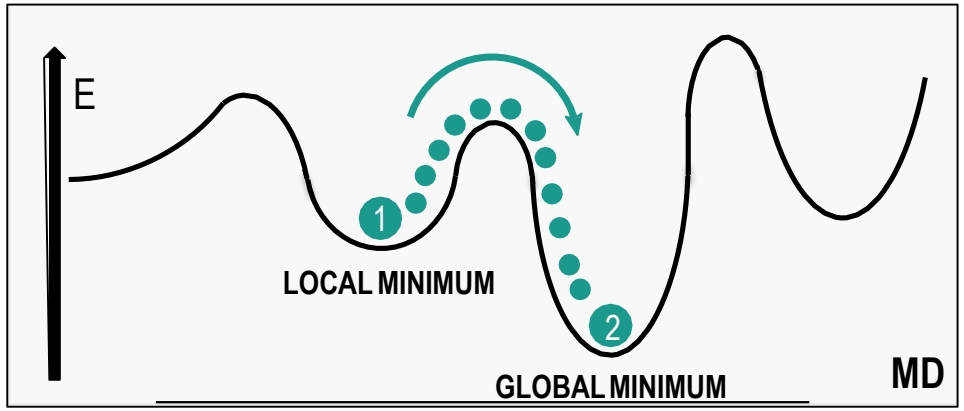
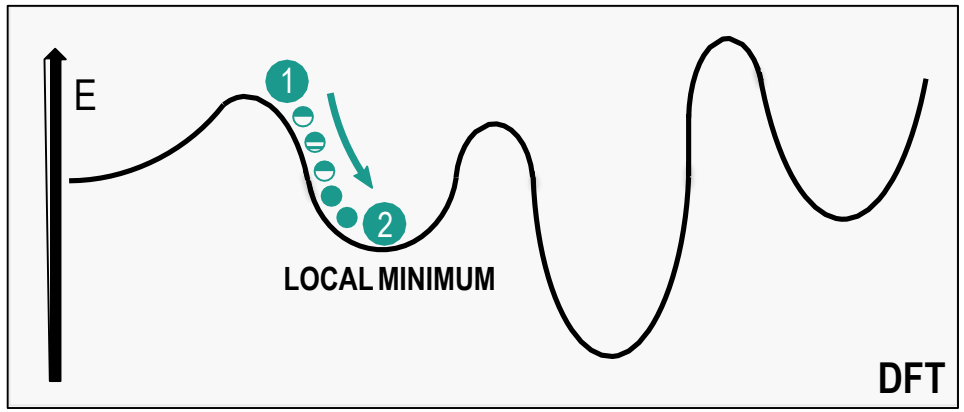
METHOD

- A combination of ***molecular dynamics*** and ***electronic structure theory*** (DFT).
- HPRC resources: 28 cores (TERRA) and 20 cores (ADA), 150 h per optimization (incl. frequency calculations).
- ***Solvent models*** and ***dispersion corrections*** were also implemented in the atomistic quantum software package Gaussian 09.





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Dr. John A. Gladysz

Dr. Lisa M. Pérez

Dr. Michael B. Hall

Andreas Ehnbom
(www.andreasehnbom.se)

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