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
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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.

Relative Stability

$X = \text{Cl} (\rightarrow)$ and $\text{Br} (\rightarrow)$

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

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SELECTED DATA • Predicting reaction outcome before performing experiments.

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- 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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