



Showcasing work from the group of Professor Elfi Kraka, Computational and Theoretical Chemistry Group (CATCO), Southern Methodist University, USA.

Metal-ring interactions in group 2 *ansa*-metallocenes: assessed with the local vibrational mode theory

This work investigates group 2 *ansa*-metallocenes by analyzing 37 distinct compounds using computational and theoretical methods, notably local mode analysis. Through the intrinsic strength of the metal-cyclopentadienyl bond, structural disparities and the influence of solvation on complex stability are revealed, while the unique effects of bridging motifs are elucidated. This computational study offers valuable insights into the role of *ansa*-metallocenes in catalysis and materials science.

As featured in:



See Juliana J. Antonio and Elfi Kraka, *Phys. Chem. Chem. Phys.*, 2024, **26**, 15143.