

A Computational Study of C-CN Bond Activation through Nickel Catalysis using the Random Phase Approximation

Craig Waitt

Montclair State University, Montclair NJ

This study evaluates the performance of a computational method known as the Random Phase Approximation (RPA) for a Nickel catalyst that activates the C-CN bond of benzonitrile. When compared to density functional theory (DFT), the RPA performs slightly better than the dispersion corrected functionals when describing the C-CN activation of benzonitrile, and slightly worse than the dispersion corrected functionals when describing the fluxionality of the reaction mechanism. However, it provides more consistent and reliable results than Møller-Plesset Perturbation Theory and Coupled-Cluster Theory with Single and Double excitations. Overall, the RPA performs on par or better than the majority of the DFT functionals and certainly performs better than the more expensive MP2. Although RPA is not error free and does not come within chemical accuracy of 1 kcal mol⁻¹, the RPA results are in excellent agreement with both accurate theoretical results and experimental data. The RPA is a step forward toward a systematic, parameter free, all-round method to describe transition-metal chemistry that offers an excellent alternative to the more expensive electron correlated methods, and less consistent DFT functionals.