Evaluation of DFT Methods for the Evaluation of Open-Shell Transition Metal Reaction Energies and Barrier Heights

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Ever since 1831 when Zeise prepared the first organometallic complex (potassium trichloro(ethylene)platinate(II)),[1] transition metal complexes have found key roles in many processes. The reaction behaviour of transition metal complexes is remarkably different from traditional organometallic complexes, and a clear understanding of their reaction mechanisms is essential. DFT has found itself as an essential tool in this endeavour, but a key question is which of the alphabet of exchange–correlation functionals to use. For closed-shell reactions, Hansen *et al*. have presented their MOR41 benchmark set of transition metal reactions[2] while I have presented my MOBH35 benchmark set of reaction energies and barrier heights.[3-4] Open-shell reactions are more complicated, yet Hansen and coworkers have reported their ROST61 benchmark set of open-shell reactions.[5] Here, I will present my latest work in benchmarking open-shell transition metal reaction energies and barrier heights, the complement to ROST61.

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