

# Catalysis of the Quadricyclane to Norbornadiene Rearrangement by $\text{SnCl}_2$ and $\text{CuSO}_4$

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*Dedicated to Professor Rolf W. Saalfrank on the occasion of his 70<sup>th</sup> birthday*

*Ab initio* and density-functional theory (DFT) calculations have been used to investigate the model rearrangements of quadricyclane to norbornadiene catalysed by single  $\text{CuSO}_4$  and  $\text{SnCl}_2$  molecules. The isolated reactions with the two molecular catalysts proceed *via* electron-transfer catalysis in which the hydrocarbon is oxidised, in contrast to systems investigated previously in which the substrate was reduced. The even-electron  $\text{SnCl}_2$ -catalysed reaction shows singlet-triplet two-state reactivity. Solvation by a single methanol molecule changes the mechanism of the rearrangement to a classical Lewis acid-base process.

*Key words:* *Ab initio* Calculations, Density Functional Calculations, Electron Transfer, Catalysis, Rearrangement