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IR spectroscopy of ferrocene and deuterated ferrocene: Experiment and theory

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The contemporary organometallic chemistry stems from the discovery of ferrocene Fe(C5H5)2, i.e., di-cyclopentadienyle iron (FeCp2 or Fc) half a century ago. Since its discovery, the heated debate whether the eclipsed or the staggered is the most stable structure of Fc continues. The fact that electronic structures and many properties of the Fc conformers are strikingly similar has been a key hurdle to differentiate or separate the configurations from one another. We recently discovered theoretically using DFT calculations that the 400-500 cm-1 region of the infrared (IR) spectra of Fc exhibits the fingerprint conformers. Such the discovery was later confirmed by IR experimental measurements in a number of solutions, in polar and non-polar solvents. Understanding of the structure and dynamics of the sandwich complex is important as Fc derivatives may inherit particular properties which only exist in one conformer such as catalysis. It is further discovered that the IR spectral fingerprint is associated with the vibrations of the centre Fe atom in the sandwich conformers, which is seen in an earlier IR experiment of Fc. As a result, we designed and conducted new high-resolution IR experiments in the gas-phase Far-IR beamline of the Australian Synchrotron to study Fc-h10 and deuterated Fc-d10. New results and analysis in gas phase and in solutions will be presented at this meeting.

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IR spectroscopy, ferrocene and it isotopes, DFT calculations

Summary

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