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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  $\text{Fe}(\text{C}_5\text{H}_5)_2$ , i.e., di-cyclopentadienyl iron ( $\text{FeCp}_2$  or  $\text{Fc}$ ) half a century ago. Since its discovery, the heated debate whether the eclipsed or the staggered is the most stable structure of  $\text{Fc}$  continues. The fact that electronic structures and many properties of the  $\text{Fc}$  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  $\text{cm}^{-1}$  region of the infrared (IR) spectra of  $\text{Fc}$  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  $\text{Fc}$  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  $\text{Fe}$  atom in the sandwich conformers, which is seen in an earlier IR experiment of  $\text{Fc}$ . 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  $\text{Fc-h}_{10}$  and deuterated  $\text{Fc-d}_{10}$ . New results and analysis in gas phase and in solutions will be presented at this meeting.

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Primary author: Prof. WANG, Feng (Swinburne University of Technology)

Co-authors: Prof. CHANTLER, Chris (The University of Melbourne); Dr APPADOO, Dominique (Australian Synchrotron); Mr ISLAM, Shawkat (Swinburne); Dr BEST, Stephen (The University of Melbourne); Mr ISLAM, Tauhid (The University of Melbourne)

Presenter: Prof. WANG, Feng (Swinburne University of Technology)

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