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Ferrocene conformers: where DFT calculations meet measurements

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As the most important organometallic sandwich compound in chemistry, ferrocene (Fc , $\text{Fe}(\text{C}_5\text{H}_5)_2$) can also serve in hydrogenases as metal catalysis in the interaction with enzyme. As a result, understanding the structural and functional details of the active site of hydrogenases through X-ray crystallography, spectroscopic and computational methods, has been the bottleneck of biomimetic and bioinspired catalysts in chemistry. However, it is important to obtain a good understanding of Fc structure as since its discovery, the heated debate whether the eclipsed (e-Fc) or the staggered (s-Fc) 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, until our recently study which discovered theoretically using DFT calculations that the 400-500 cm^{-1} region of the infrared (IR) spectra of Fc [1] exhibits the fingerprint conformers, which is seen in an earlier IR experiment of Fc. Such the discovery was later confirmed by IR experimental measurements in a number of solutions. In this presentation, we discuss the design and conduction of a series of new high-resolution IR experiments in the gas-phase and solid phase under various temperatures at the Far-IR beamline of the Australian Synchrotron to study the IR for Fc and deuterated Fc-d10. Preliminary results and analysis will be presented at this meeting.

1. Mohammadi, N. et al, J. Organomet. Chem., 213(2012)51-59.

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