Contribution ID: **63** Type: **Contributed talk**

Hydrogen-Bond-Mediated Conformational Locking and Quantum Tunnelling Effects in a Ferrocene Based Molecular Rotor

Thursday 18 September 2025 10:30 (20 minutes)

Despite being driven by quantum processes, most synthetic molecular machines exhibit classical kinetics, whereas operation by quantum tunnelling is largely elusive. In a recent investigation into the dynamics of metallocene molecular rotors, we found evidence of quantum tunnelling effects in the rotational spectrum of 1,1'-ferrocenedimethanol. Metallocenes are organometallic compounds with two nearly parallel rings surrounding a central metal atom. The simplest and best-known example of this group of sandwich compounds [1] is ferrocene, where two cyclopentadienyl rings freely rotate around a central Fe(II) atom, adopting staggered or eclipsed configurations. The rotational behaviour and associated energy barrier of these molecules depends on the substituents introduced to the rings. Bulky groups tend to increase the rotational barrier, often locking the molecule into specific configurations [2]. However, in some cases, such as phenyl substitution, unexpected effects like concerted ring rotation can occur [3].

In this contribution, we discuss a topology where a hydrogen bond between hydroxymethyl groups locks the system into a staggered or eclipsed configuration. We present experimental data from jet-cooled broadband rotational spectroscopy and discuss theoretical strategies used to interpret the observed tunnelling effects using complementary quantum chemistry calculations.

References
[1] Browne, W. R.; Pijper, D.; Pollard, M. M.; Feringa, B. L.; Synthetic Molecular Machines, based on noninterlocked molecules; from concepts to applications. Solvay Conference. Wiley, 2008.
[2] Luke, W.D.; Streitweiser, A.; J. Am. Chem. Soc., 1981, 103, 3241–3243.
[3] Castellani, M.P.; Wright, J.M.; Geib, S.J.; Rheingold, A.L.; Trogler, W.C.; Organometallics, 1986, 5, 1116–1122.

Keywords

Hydrogen bond: strong, State of system: gas, Metallocenes, Rotational Spectroscopy, Quantum Tunneling, Molecular Rotors

This abstract is submitted for....

HBond 2025 conference

Primary authors: CAMPOS, Nuno (CFisUC); ROQUE, Rita (CFisUC); VIEIRA, Ricardo (CFisUC); DOMINGOS, Sérgio (CFisUC)

Presenter: CAMPOS, Nuno (CFisUC)