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Low temperature IR spectra of frozen solutions of Ferrocene – The meeting place of experiment and theory?”

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While the measurement of low-temperature spectra of “isolated molecules” can be achieved by the use of noble-gas matrices, a simpler method using paraffin wax has been applied to the preparation of samples of ferrocene (Fc) for cryogenic IR spectroscopy. By control of the solute concentration it has been possible to achieve spectra characteristic of those obtained from RT solutions in non-coordinating solvents where the wax samples have the advantage of being suitable for low temperature measurements, avoiding further crystallisation during cooling.

The key IR bands sensitive to the conformational form of Fc are found to have a complicated temperature dependence that provides information on the conformational distribution of the species and the shape of the potential energy surface. Importantly, the low temperature spectra give a pattern of IR bands in excellent agreement with calculation (band splitting and intensities). The study has implications both in terms of the conformational analysis of the archetypal organometallic arene, Fc, but also the relationship between the calculated and observed IR spectra of molecules with low energy conformational barriers.

Keywords

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