WETTING FERROCENE AS A WAY TO INVESTIGATE ITS GAS PHASE STRUCTURE BY ROTATIONAL SPECTROSCOPY

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In ferrocene ($Fe(C_5H_5)_2$), the first discovered metallocene, iron is sandwiched between two cyclopentadienyl rings in an eclipsed configuration. Ferrocene is an orange solid that sublimates easily and is stable at high temperatures. Due to its symmetry (D_{5h}) this compound does not have a dipole moment, so it is not active in the microwave region and consequently, its gas phase structure is not accessible through microwave spectroscopy. However, as it has been shown for triacetone triperoxide [1], its complexation with water makes it possible. In this work, we have done a combined theoretical and experimental work to observe and analyze the microwave spectrum of ferrocene – H_2O. The theoretical computations predict two possible low-energy structures of the complex. In one form, water lies in the σ_h plane of ferrocene. In the other form, water is close to the C_5 axis of ferrocene on top of one of the cyclopentadienyl rings. Both forms have been observed. The most intense spectrum is that of a symmetric top with satellite patterns consistent with the effects of the free rotation of water. The rotational constant B determined for this spectrum is close to that predicted for the second axial form so that we can conclude that water is located along the C_5 axis and freely rotating around it. This motion averages the ferrocene – H_2O structure to that of a symmetric top. Different isotopic species have been detected, including ^{54}Fe and ^{13}C in their natural abundances, which have made it possible to determine the structure of the heavy atom skeleton of ferrocene and the axial location of water. A second weaker rotamer with an asymmetric top spectrum has rotational constants very close to those predicted for the other ferrocene-water conformer. Experimental and theoretical work is still in progress.

1. Blanco, S.; Macario, A.; Garcia-Calvo, J.; Revilla-Cuesta, A.; Torroba, T.; Lopez, J.C.; Microwave Detection of Wet Triacetone Triperoxide (TATP: Non-Covalent Forces and Water Dynamics. Chem. Eur. J. 2021, 27, 1680–1687.