CALCULATIONS AND GAS PHASE MEASUREMENTS OF THE COMPLEX FORMED WITH FERROCENE AND HCL

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Calculations for the Ferrocene and HCl complex using MP2/6-31+G(d) on C,H,Cl and Hay-Wadt VDZ (n+1) core potential on Fe indicate preferred binding of HCl along the b-axis of ferrocene, with hydrogen pointing to Iron. Several transitions have been measured using a Flygare-Balle microwave spectrometer in the 4-12 MHz range showing chlorine quadrupole splitting consistent with the complex. The calculated structure and quadrupole coupling constants will be presented with recent progress on measurements.