Hyperfine Interactions of Muoniated Ethyl Radical in Supercritical CO_2

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The muoniated ethyl radical was studied in supercritical carbon dioxide. The Hyperfine coupling constants were measured over a range of temperatures from 305 K to 475K, with the density of CO_2 being held constant at 0.25, 0.42 and 0.7 (g/cm^3). The system was modeled with DFT calculations at UB3LYP level and with 6-311++g(2df,p) basis set for optimization, frequency calculations and for single point calculations. There is a decrease in the hyperfine coupling constants as a function of density. This can be attributed to the interaction between the CO_2 molecule and the p-orbital of the ethyl radical generated from the addition of muonium. This effect also has an effect on the values associated with the hyperfine coupling constants associated with the α-proton and β-proton.

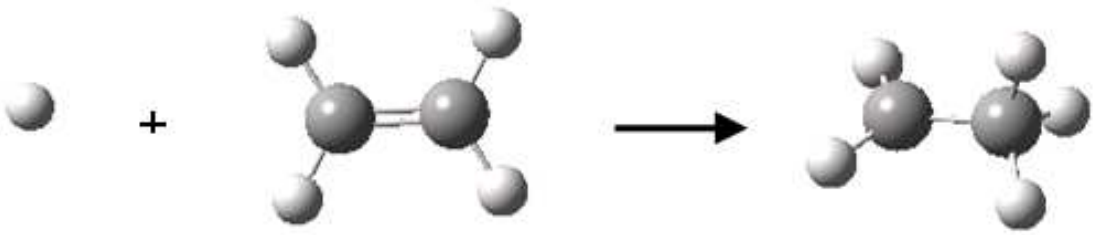

Fig. 1: reaction scheme for addition of muonium to ethane.