586f Decomposition Kinetics of Diethylzinc by Quantum Chemical Calculations

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The gas-phase decomposition of diethylzinc, a common precursor for deposition of Zn-VI compounds, was studied. First principles quantum calculations were employed to describe the bond dissociation behavior and the model-chemistry B3LYP/6-311G(d) was selected based on comparison to previously reported bond dissociation energies. The thermodynamic properties were estimated using this model to compare the equilibrium conversions. The B3LYP/6-311G(d) model chemistry revealed that the major pathway for the gas-phase homogeneous pyrolysis of diethylzinc is ß-hydride elimination. Reasonable transition states during ß-hydride elimination were envisioned and the modeled energies and thermodynamic properties were used to identify probable reaction steps. Vibrational frequencies of reaction intermediates and products were computed along with calculation of the Zn-C symmetrical motions. These values were used to assist in the interpretation of gas phase Raman scattering experiments. In addition that, FEM hydrodynamic simulation revealed that simple bond dissociation between zinc and carbon atoms is also presented in gas phase. The kinetic study for two competing reactions was performed and formation and decomposition chemistry of reaction intermediates were examined using quantum chemical calculation and Raman spectroscopy.