Kinetics of Bimolecular Decomposition Reactions of Molybdenum-hexachloride

Jovan Livada, Deacon Lile, George Shields, Karl Kirschner

We have used Gaussian ’03 package to obtain thermodynamic data of the decomposition reactions of Molybdenum chlorides. The reactions look like this:

$$MoCl_x + H \Rightarrow MoCl_{x-1} + HCl \quad (x=6,5 \ldots 1)$$

Once the thermodynamic data were obtained, we used professor Truong’s program “Computational science and engineering online” to generate kinetics data. This program uses Gaussian thermodynamic data to find the Arrhenius parameters, forward and reverse rates of the reaction. We found the thermodynamic data via Gaussian '03 with the B3LYP level of theory for optimizations and frequencies, and the CCSD(T) level of theory for single point energy calculations. We used two different basis sets that incorporate the ECP (effective core potential) the LanL2DZ and the SDD basis sets. We imported the values of the reactants, products, transition states and the values of IRC jobs, into the kinetics program. We ran Simple transition state theory (TST) with Eckart Tunneling. We found the Arrhenius parameters, reverse, and forward rates for all reactions. The results have shown forward rates of around 10e-12 order of magnitude. The reaction of $MoCl_4$ with the hydrogen gas radical produced the fastest rates at about 10e-4 order or magnitude at 300K.