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Title: Pressure dependence in the competitive thermal isomerization /decomposition of the cyclohexyl radical

Abstract:

Cyclohexane and alkylated cyclohexanes comprise a large portion of many transportation fuels. Under certain conditions these compounds readily undergo subsequent dehydration reactions to aromatic molecules like benzene and toluene.  Although the mechanism is well known, little attention has been given to the pressure dependence of these reactions. One of the first steps in cyclohexane dehydration to benzene is H-elimination from cyclohexyl.  RRKM/Master Equation calculations were carried out to probe the pressure dependence of competitive thermal isomerization/decomposition in the cyclohexyl system.  The results reveal rich distribution of products highly dependent on both temperature and pressure. Cyclohexene production is increasingly favored with lower pressure and increasing temperature. The role of pressure dependence on predicted benzene mole fractions is also discussed in the context of various flame conditions.