High Level *Ab initio*, DFT and RRKM Calculations for the Unimolecular Decomposition Reaction of Ethylamine

M. Almatarneh[1]*, M. Altarawneh[2], R. Poirier[3] and I. Saraireh[4]

[1]*General Studies Department, Jubail University College, Jubail Industrial City, Saudi Arabia*
[2]*Department of Chemical Engineering, Al-Hussein Bin Talal University, Ma'an, Jordan*
[3]*Department of Chemistry, Memorial University, St. John's, Canada*
[4]*Department of Chemical Engineering, Al-Hussein Bin Talal University, Ma'an, Jordan*

*Author for correspondence e-mail: matarnehm@ucj.edu.sa

The mechanism for the decomposition reaction of ethylamine, $CH_3CH_2NH_2$, was investigated using high level *ab initio* and DFT calculations. Optimized geometries were fully optimized at MP2 and B3LYP levels of theory using 6-31G(d) and 6-31+G(d) basis sets. Single point energies were determined at G3MP2B3 and G3B3 levels of theory. Thermodynamics properties, activation energies, enthalpies and free energies of activation were calculated for each reaction pathway investigated. Intrinsic reaction coordinate (IRC) analyses were performed to characterize the transition states on the potential energy surface. The conformational interchange in ethylamine has been examined. We were interested in the first stage-cracking pattern postulated for the decomposition of ethylamine. Therefore, four pathways for the decomposition reaction of ethylamine were studied. All pathways involve a 1,2-elimination reaction and 1,3-proton shift to produce ethene, ethanimine, ethenamin, and methanimine. All pathways involve a one-step mechanism. The activation energy for the most plausible pathway is 280 kJ mol^{-1} at G3MP2B3 level of theory. The results and the mechanisms for these reactions will be presented and discussed.