Calculating the Transition State of the Peptide Bond in the Ribosome

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Abstract: Based on the biology of ribosomes and amino acids within the human body, it was known that peptide bonds are what hold amino acid chains together. The purpose of this experiment was to find a transition state of the reaction within the ribosome that creates the peptide bond while keeping in line with known biological data. A P site and an A site tRNA molecule was taken, prebuilt, from the Protein Data Bank and modified slightly to correspond with what an actual reaction would look like. The structure was optimized using Gaussian, B3LYP/3-21G on the North Carolina High School Computational Chemistry Server and then run for Vibrational Frequencies to find the single imaginary frequency. Once that was found, the molecule was run under IRC calculations, both forward and reverse, to eventually find the activation energy of the energy. As a result of all the calculations, it was found that a transition state was able to be found that still supported biological fact, meaning the tRNA molecules still rotated around the 2-fold symmetry axis, and in the end, the P site tRNA was released, as it would be in a normal reaction. The reaction was found to be exothermic with an activation energy of .39 kcal/mol.

Keywords: peptide bond | ribosomal tRNA | 2-fold symmetry axis | transition state | activation energy | Gaussian | amino acids