The computational software package *Gaussian* was used with the M06 method and 6-311++g (2d,p) basis set to investigate the tautomers of biacetyl, particularly the keto-enol tautomerization. All the tautomers' structures for singlet biacetyl were generated and their geometries were optimized. The optimized geometries were then examined to determine which conformations were more stable and lower in energy. The vibrational calculations were then performed and energies calculated. The transition state of biacetyl to each tautomer was calculated and optimized. The pathway of the reaction was calculated using the transition state calculations. The reaction pathway calculation produced reaction coordinate graphs and allowed the energies of activation to be calculated. The reaction coordinate graphs and energies of activation were then used to analyze each biacetyl to tautomer reaction, and compare the energy barriers for each reaction. The data showed that 2-oxo-3-oxoniobutan-1-ide had the lowest energy barriers of all the tautomers. The tautomer with the highest energy barrier was 3-oxobutan-4-id-2-olate but only some of its conformations were extremely high in energy.