Triacetone triperoxide (TATP) has been prepared in order to study the effect of pH and temperature on the reaction kinetics. Raman spectra of liquid mixtures of acetone and hydrogen peroxide were recorded versus time throughout the experiments. The spectral data of the liquid phases indicate that at 25 degrees C the reaction between acetone and hydrogen peroxide proceeds to form intermediates within one day. Based on the assumption that a likely reaction path involves a sequence of reaction steps between acetone and hydrogen peroxide, calculations of Raman spectra were performed using a density functional theory (DFT)/Hartree-Fock approach. It was not possible from this to assess with certainty which intermediate products formed most extensively in an acetone/hydrogen peroxide mixture. However, it was concluded that the most likely reaction mixture is a mixture of the different intermediate products and that the rate determining step is the ring closure. The reaction rate of TATP formation was found to increase with temperature and with sulfuric acid additions to the acetone/hydrogen peroxide mixture. By correlation of the induction time of TATP crystallization against pH it was shown that the reaction rate is first order with respect to the H+ concentration. Raman spectra of the precipitates from mixtures were in agreement with previous studies done for TATP, except in one case in which a crystal crystallized at 343 K had a distinctly different Raman spectrum. Comparison with calculated spectra revealed that the crystal produced could be diacetone diperoxide (DADP) or tetraacetone tetraperoxide (TrATrP). Single crystal X-ray diffraction analyses revealed that the crystal crystallized at 343 K was DADP.