This bachelor thesis deals with the study of the vibrational spectra of melamine and thiram molecules using methods of Raman spectroscopy. Quantum chemical simulations are then used for a detailed interpretation of the measured spectra. Melamine is used as an industrial chemical in plastics and adhesives. However, its ingestion can lead to urinary bladder or kidney stones and, in extreme cases, cause death. Thiram is used as a fungicide and animal repellent, but it is toxic. The investigations included the variability of the Raman spectra of both contaminants in the polycrystalline and liquid phase and the spectra obtained by using the drop coating deposition Raman spectroscopy at different concentrations.