VIBRATIONAL ANALYSIS OF 1,3,3-TRINITROAZETIDINE USING MARIX ISOLATION INFRARED SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS.

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Infrared spectra of 1,3,3-trinitroazetidine (TNAZ), $(O_2N)_2C(CH_2)_2NNO_2$, were obtained using FTIR detection of samples evaporated from a Knudsen Cell and codeposited with argon on a 15K IR window. Spectra of matrix isolated TNAZ and isotopically labeled TNAZ are used to assign 24 of the 45 fundamental molecular vibrations. Comparisons among experimental spectra and spectra calculated using Hartree-Fock, second-order Moller-Plesset theory (MP2) and three density functional theory (DFT) methods indicate that DFT gives a more accurate vibrational description than MP2 or HF. Three pairings of exchange and correlation functionals were employed in comparing DFT results. First, Becke's 88 exchange was used with Perdew's 86 correlation functional (BP86). Next, Becke's three-parameter hybrid method was combined with Perdew's 86 correlation functional (B3P86) to permit comparisons to the BP86 method. Finally, Becke's three parameter hybrid was used with the Lee-Yang-Parr correlation functional (B3LYP). Overall, best results were obtained with BP86 and B3LYP.