HIGHLY ACCURATE VIBRATIONAL TRANSITION ENERGIES FOR THE HIGH ENERGY DENSITY MATERIAL TETRAHEDRAL N_4

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More than a decade ago, tetrahedral (T_d) N_4 was suggested as a potential high energy density matrial, which could be used as a novel rocket fuel, among other possible uses. However, the only report of its possible synthesis was inconclusive, partly because the isotopic shifts found in the matrix isolation experiment did not agree well with theoretical values obtained from harmonic frequencies. In this study we have re-examined the theoretical spectroscopy of T_d N_4 using very high levels of theory and by computing a full quartic force field. Vibrational frequencies obtained from this new force field, together with isotopic shifts, will be reported. As a by product of this study, we have also computed a new more accurate heat of formation for T_d N_4 which confirms its potential as a high energy density material.