THE ELECTRONIC STATES AND VIBRATIONAL FUNDAMENTALS OF THE NITRIC OXIDE DIMER, $(NO)_2$, AND DIMER CATION, $(NO)_2^+$

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The weakly-bound nitric oxide dimer, with dissociation energy $D_0 = 2.1$ kcal mol^{-1}, is over 7 times more strongly bound than the carbon monoxide dimer, due to unusual partial covalent bonding. Using CASSCF and MRCISD calculations, the lowest 8 states are computed to lie within a 1 eV span, corresponding to electronic excitations in the *infrared.* As well, coupled-cluster CCSD(T) calculations of the vibrational fundamentals of $(NO)_2$ and $(NO)_2^+$ were performed, which aided both (i) the spectroscopic detection of the previously unknown gas-phase fundamentals of the neutral, and (ii) the interpretation of the ZEKE photoionization spectrum obtained a few years ago.