The Jahn Teller and pseudo-Jahn Teller effect in the dark $\tilde{A}$ state of the nitrate radical NO$_3$ KANA TAKEMATSU, DAVID ROBICHAUD, MITCHIO OKUMURA, Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, CA 91125, JOHN STANTON, Department of Chemistry, University of Texas, Austin, TX 78712 — Despite its apparent simple molecular structure, the lowest electronic states of the nitrate radical NO$_3$ remain poorly understood. In particular, the three lowest states of the radical provide a benchmark for testing models of the Jahn-Teller (JT) and pseudo-JT effects. The dark $\tilde{A}$ state of NO$_3$ undergoes strong JT distortion, suggesting that models with only linear and quadratic vibronic couplings are inadequate. We present cavity ringdown (CRD) and integrated cavity output (ICOS) spectra of the forbidden $\tilde{A}^2E' \leftarrow \tilde{X}^2A'_2$ transition (preliminary report in Deev, et. al. J.Chem. Phys., 2005. 122:224305) and compare them to a simulation based on a model Hamiltonian developed by Koppel, Domcke and Cederbaum that incorporates both JT and PJT couplings. New insights into the pseudo-JT effect among the lowest states are gained by examination of intensity-borrowing mechanisms for the observed vibronic bands.

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