Supporting Information: The $\tilde{A} - \tilde{X}$ Absorption of Vinoxy Radical Revisited: Normal and Herzberg-Teller Bands Observed via Cavity Ringdown Spectroscopy

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December 17, 2009

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Table 1: Unscaled harmonic and fundamental frequencies calculated at the UB3LYP/aug-cc-pVTZ level, and unscaled harmonic frequencies calculated at the UCCSD/cc-pVDZ level for $\tilde{X}$ and $\tilde{A}$ state equilibrium structures of vinoxy. The number in bold at the head of each column is the zero point energy. All values are in cm$^{-1}$.

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Table 2: (Squared) values of Duschinsky rotation matrix elements. Rows and columns are indexed by $\tilde{X}$ and $\tilde{A}$ state frequencies (cm$^{-1}$), respectively. Duschinsky matrices have been computed in the harmonic approximation but are indexed by unscaled fundamental frequencies (B3LYP/aug-cc-pVTZ) and unscaled harmonic frequencies (CCSD/cc-pVDZ).

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Table 3: Electronic energies (a.u.) and cartesian coordinates (Å) for equilibrium and vibrationally averaged structures of vinoxy.

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Table 4: Input parameters used for simulations of the rotational contours of vinoxy. Rotational constants were obtained from the anharmonic vibrationally-averaged structures calculated at the UB3LYP/aug-cc-pVTZ level; all spin rotation parameters are set to the $\tilde{X}$ state values experimentally determined by Endo and Hirota.\(^1\)

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Control parameters

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