

INSIGHT INTO THE JAHN-TELLER EFFECT IN THE NITRATE RADICAL VIA THE A-X HOT BANDS

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Elucidation of the electronic states of the nitrate radical NO_3 remains an interesting puzzle for experimentalists and theorists alike. The A^2E'' state is Jahn-Teller active and is pseudo-Jahn-Teller coupled to the ground X^2A_2' and excited B^2E' states. Analysis of the vibronic-allowed A-X transition spectrum shows vibronic bands exhibiting both static and dynamic distortions depending on the vibrational level of the upper A state. In the $E''x e' = a_1'' + a_2'' + e''$ manifold, only the a_1'' levels are accessible under ambient temperature experiments. We have gained new insight into the A state by examining the hot bands of NO_3 , as previously dark levels of the A state become accessible. We present analysis of our hot band spectrum along with calculations of the upper A state levels.