

A THEORETICAL PREDICTION OF ELECTRONIC TRANSITIONS IN C_3

DAVID W. SCHWENKE, GALINA M. CHABAN, *NASA Ames Research Center, Moffett Field, CA 94035.*

We have carried out first principle calculations of electronic transitions in C_3 . Low lying electronic states have linear or near linear minima, and thus are characterized by $D_{\infty v}$ symmetry labels. The ground state has $^1\Sigma_g^+$ symmetry, and can be reasonably treated by triatomic bound state codes that assume the Born-Oppenheimer approximation is valid. The lowest excited state has $^1\Pi_u$ symmetry, and explicit coupling between electronic and nuclear angular momentum must be considered: the Renner-Teller effect. We treat this coupling exactly so our results are independent of the choice of coordinates. Furthermore, the $^1\Pi_u$ state is perturbed by the lowest triplet state, and we include this coupling as well.