

# INTENSITY CALCULATIONS FOR THE $\tilde{A}^1A_u(C_{2h}) - \tilde{X}^1\Sigma_g^+(D_{\infty h})$ TRANSITION OF ACETYLENE

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The  $\tilde{A} - \tilde{X}$  transition of acetylene was the first electronic transition for which a change of point group was confirmed in detail<sup>a</sup>. Previously, harmonic Franck-Condon calculations for this transition were presented<sup>b</sup>. The present calculations allow for anharmonicity in the ground state, although the upper-state potential is still assumed to be harmonic<sup>c</sup>. The transition moment is taken to be proportional to the  $q_4''$  bending coordinate. For the calculation of the dispersed fluorescence spectrum<sup>d</sup> it is found that the global potential surface of Halonen, Child and Carter<sup>e</sup> gives the best qualitative agreement for the intensities, but could be improved for the energies of high bending states.

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<sup>a</sup>C. K. Ingold and G. W. King, *J. Chem. Soc.*, 2702–2755 (1953); K. K. Innes, *J. Chem. Phys.* **22**, 863–876 (1954).

<sup>b</sup>J. K. G. Watson, Paper TG11, OSU Symposium (1998).

<sup>c</sup>J. D. Tobiasson, A. L. Utz, E. L. Sibert III, and F. F. Crim, *J. Chem. Phys.* **99**, 5762–5767 (1993).

<sup>d</sup>M. P. Jacobson, Ph.D. Thesis, Massachusetts Institute of Technology (1999); M. P. Jacobson and R. W. Field, *J. Phys. Chem.* **104**, 3073 (2000).

<sup>e</sup>L. Halonen, M. S. Child, and S. Carter, *Mol. Phys.* **47**, 1097 (1982).