FRANCK-CONDON 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 (1,2). This paper presents harmonic calculations of intensities of the vibrational structure of this transition, using the force field of Tobiason *et al.* (3) for the $\tilde{A}$ state. The $\tilde{A} - \tilde{X}$ transition correlates with the forbidden ${}^1\Sigma_u^- - {}^1\Sigma_g^+$ at linear geometries, and the transition moment is assumed to be proportional to the q_4'' bending coordinate. There are difficulties in the calculation because the usual harmonic wavefunctions of the upper state do not behave correctly at linear geometries. To correct this, a different calculation would have to be done for each K_a-value. Approximate results for the intensity integrals are presented. These agree well with measured values for the $v_3' - 0$ bands in the absorption spectrum with v_3' up to 5 (1), but the agreement is only qualitative for recently measured emission bands (4) which peak near $v_4'' \approx 14$, and must be seriously affected by anharmonicity.

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