INTENSITY CALCULATIONS FOR THE $\tilde{A}^1 A_u(C_{2h}) - \tilde{X}^1\Sigma_g^+(D_{\infty h})$ 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[a]. Previously, harmonic Franck-Condon calculations for this transition were presented[b]. The present calculations allow for anharmonicity in the ground state, although the upper-state potential is still assumed to be harmonic[c]. The transition moment is taken to be proportional to the q_4'' bending coordinate. For the calculation of the dispersed fluorescence spectrum[d] it is found that the global potential surface of Halonen, Child and Carter[e] gives the best qualitative agreement for the intensities, but could be improved for the energies of high bending states.

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