CALCULATING FRANCK-CONDON FACTORS FOR TRANSITIONS FROM LINEAR TO BENT STATES: APPLICATION TO THE ELECTRONIC SPECTRUM OF DIACETYLENE

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Expressions will be presented for calculating Franck-Condon factors in the harmonic approximation for transitions from a linear ground state to a bent excited state. These expressions are similar to those published previously by Doktorov et. al.[a] for the case where the number of modes does not change between the two states. The derivation of these equations will be briefly discussed. They will be applied to several test cases, including electronic transitions in diacetylene, C_4H_2.

[a] J. Mol. Spec., 64, 302-326 (1977).