FERMI RESONANCE PERTURBATIONS OF ORBITAL ANGULAR MOMENTUM (RENNER-TELLER) COUPLING IN TRIATOMIC MOLECULES: THE STRETCH-BENDER APPROACH

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Fermi resonance effects on Renner-Teller coupling in NH_2 and CH_2 have been identified. We have developed an extension of the semi-rigid bender approach of Jungen and Merer[b] and of Duxbury and Dixon[c] to calculate the interplay between Renner-Teller and vibrational resonances in detail. The basic idea is that if in the semi-rigid bender the bond length relaxes to follow the minimum on the potential energy surface, the effect of the stretch-bend coupling should be minimised in this basis. This should simplify the calculations compared to those using a full three dimensional basis when only a few quanta of the stretching vibrations are excited via resonances. The effects of the interplay between Renner-Teller and vibrational coupling will be discussed using some of the most recent data[d] obtained for the $\tilde{b}$ state of CH_2, making use of two-dimensional wavefunctions without and with Fermi resonance effects.

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