RENNER-TELLER AND SPINORBIT COUPLING IN H_2S+ AND AsH_2

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The semi-rigid bender approach of Dixon and Duxbury,[a] and the alternative approach by Jungen and Merer[b] were devised to minimise the effects of the large amplitude bending upon the Renner-Teller interaction. They also allow the effects of large amplitude motion on the rotational structure to be calculated, including the switchover from bent to linear behaviour. From this the stretch-bender reference-frame [c] were developed to allow the separation of large amplitude bending motion and symmetric stretching. It has been used to calculate vibrational resonances, the effects of spin-orbit coupling, and of overall rotation. As both states are derived from the degenerate π state of the linear molecule, we wish to show the utility of this approach to understanding the large interaction between the high lying bending levels of the the electronic ground state and the low lying levels of the excited state, including the predissociation of higher vibronic levels, of H_2S+ and AsH_2.

[a] Molec. Phys. 43,255(1981)
[b] Molec. Phys. 40,1(1981)
[c] J. Chem. Phys. 108,2336 (1998) and J. Mol. Spectrosc. 211,7 (2002)