RENNER-TELLER COUPLING IN H_2S+: PARTITIONING THE ROVIBRONIC AND SPINORBIT COUPLING HAMILTONIAN

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The stretch-bender reference-frame[a] was 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. Its use allows the block factorisation of the Renner-Teller interaction matrix. We wish to show the utility of this approach when two different approaches by Dixon and Duxbury,[b] and Jungen and Merer[c], are used to minimise the effects of the large amplitude bending upon the Renner-Teller interaction. It also allows the effects of large amplitude motion on the rotational structure to be calculated, including the switchover from bent to linear behaviour.

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