Laser Spectroscopic Study of CaH B/B'(v=10, 11) -X bands

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Electric transitions of Calcium monohydride (CaH) have been found in sunspots and M dwarf stars [1], and have been used to investigate them. Despite the long history of study of this molecule the first two exited $^2\Sigma^+$ states, B/B' and $D^2\Sigma^+$, have continued to pose challenges for experiment and theory. The B/B' state is formed by the avoided crossing between two diabatic states and a non-bonding diabatic state, resulting in a double minimum potential energy function. Martin calculated energy levels in Born-Oppenheimer approximation [2]. He was able to perform a least-squares fitting to the available rovibronic data. The result was a set of empirically generated, but physically-constrained, potential energy curves for the X, B/B', D states. Carlsund-Levin et al. used updated versions of Martin's potential but also accounted for Martin's R-dependent interaction term in a coupled-channel (CC) calculation of the rovibronic energies [3]. In a bid to resolve discrepancies in vibronic assignments of these states we observed the rotational-resolved fluorescence spectrum of CaH.

In previous work, we observed four vibronic levels and attributed them to B/B' (v=12, 13, 14 and 16) lying above the double-minimum potential energy barrier, and five levels previously assigned to the D state [4], to the B/B' state. In additional to this, we recently observed the B/B' (v=10, 11) levels. Fig 1 shows the vibrational levels of D and B/B'. The levels' properties alternate strongly with vibrational excitation and the new assignment brings the experimental vibronic structure into remarkably good agreement with the CC calculation values of Carlsund-Levin.

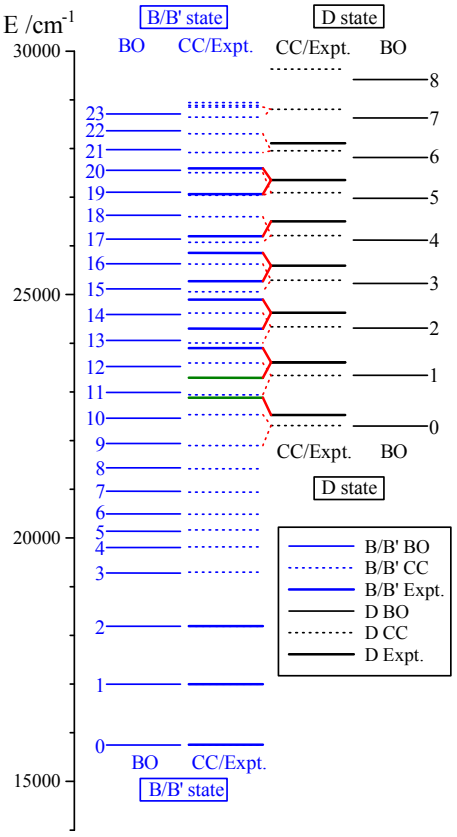

Figure 1: Vibronic energy levels of the B/B'$^2\Sigma^+$ and $D^2\Sigma^+$ states of CaH. Outer lines show values calculated in the Born-Oppenheimer approximation [2]. Dotted lines in the center show the couple-channel (CC) calculated values [3]. Thick solid lines in the center show experimental values [4-7]. B/B' (v=10, 11) are shown by the green lines. Close lying levels are connected (in the center) to highlight interactions between the B/B'$^2\Sigma^+$ and $D^2\Sigma^+$ states.

References

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