LOW-LYING 0⁺ STATES OF BISMUTH HYDRIDE

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Test calculations for BiH 0^+ ground and excited states using a CI configuration selection procedure, including the effective spin-orbit operator in the selection process (intermediate coupling CI), are compared with previous work in which the spin-orbit operator was included only in a final CI over λ -s selected configurations. While the lowest states are well described by the latter procedure, our results show an error in the previous work in an upper state due to the failure to detect a charge transfer avoided crossing in their final intermediate coupling CI.