ACCURATE *AB INITIO* POTENTIAL ENERGY SURFACE AND PREDICTED SPECTROSCOPIC PROPERTIES OF BeH_2, BeD_2 and BeHD

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A three-dimensional potential energy surface for the ground electronic state of BeH_2 has been constructed from more than 6800 symmetry-unique *ab initio* points calculated at the icMRCI/aug-cc-pV5Z level, and corrected for core electron electron correlation computed at the MR-ACPF/cc-pCV5Z level. Calculated spectroscopic constants of BeH_2 and BeD_2 are in excellent agreement with recent experimental results, and spectral constants for BeHD are predicted using the same potential surface. The effect of different interpolation methods on predicted potential function values and on the calculated level energies and spectroscopic constants has been examined. Preliminary results of work on determining a global analytic function for this three-dimensional potential energy surface based on symmetric and antisymmetric stretching coordinates will be described.