

THEORETICAL STUDIES OF THE ELECTRONIC STRUCTURE OF THE GROUND AND LOW-LYING EXCITED STATES OF ScH_2^{++} , TiH_2^{++} , VH_2^{++} , CrH_2^{++} , and MnH_2^{++}

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In all of the titled molecules the two positive charges remain localized essentially on the transition metal and the low-lying electronic states are those of the corresponding dipositive free ion split by a virtually intact, polarized H_2 molecule. We discuss the character of these states, their binding energy, and the splitting of the free ion term as determined by high level ab-initio calculations.