

## THE ELECTRONIC STRUCTURE OF ScH<sup>++</sup>, TiH<sup>++</sup>, VH<sup>++</sup>, CrH<sup>++</sup>, AND MnH<sup>++</sup>

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We will discuss the electronic structure of the ground and low-lying excited states of the titled transition metal hydrides. Of these ScH<sup>++</sup>, TiH<sup>++</sup>, and VH<sup>++</sup>, are thermodynamically stable while CrH<sup>++</sup>, and MnH<sup>++</sup> are expected to be very long lived. While the charge distribution for each molecule is approximately M<sup>+1.85</sup> H<sup>+0.15</sup> the nature of the bonding changes very rapidly from a conventional sigma bond in ScH<sup>++</sup>, to what may be described as an antiferromagnetic coupling of the Mn<sup>++</sup> ion to the H atom in MnH<sup>++</sup>. We will discuss trends in  $D_e$ , bond lengths and vibrational frequencies and will compare with the corresponding neutral and monovalent hydrides.