MULTI-REFERENCE CONFIGURATION INTERACTION CALCULATIONS OF THE LOW-LYING ELECTRONIC STATES OF IRON AND VANADIUM MONOHYDRIDE, FeH and VH

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We have carried out *ab initio* multi-reference configuration interaction (MRCI) calculations of the low-lying electronic states of iron and vanadium monohydride, FeH and VH. The purpose of the FeH study was to calibrate our methodology against the large body of experimental data on that system[b] in order to make reliable predictions about the relatively unknown spectrum of VH.[c] We employed a Bauschlicher-ANO(spdfg) basis for Fe and V, and an aug-cc-pVTZ basis(spd) for H. The MRCI consisted of internally contracted single and double excitations from the wavefunction resulting from a complete active space MCSCF calculation involving the six or nine valence electrons and the ten valence orbitals (4s, 3d, 4p) plus an additional four virtual orbitals, i.e., a CAS(6,14) or CAS(9,14) reference function. Here we report the calculated electronic properties, including dipole moments, and spectra of these molecules.

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[b]See, for example, W.J. Balfour, J.M. Brown, and L. Wallace, *J. Chem. Phys.* **121**, 7735 (2004) and references therein.

[c]S.P. Walch and C.W. Bauschlicher, Jr., *J. Chem. Phys.* **78**, 4597 (1983).