Supporting Information for

"Structural and Electronic Properties of Hydrated V_nH_2O and $V_n^+H_2O$, $n \leq 13$, Systems"

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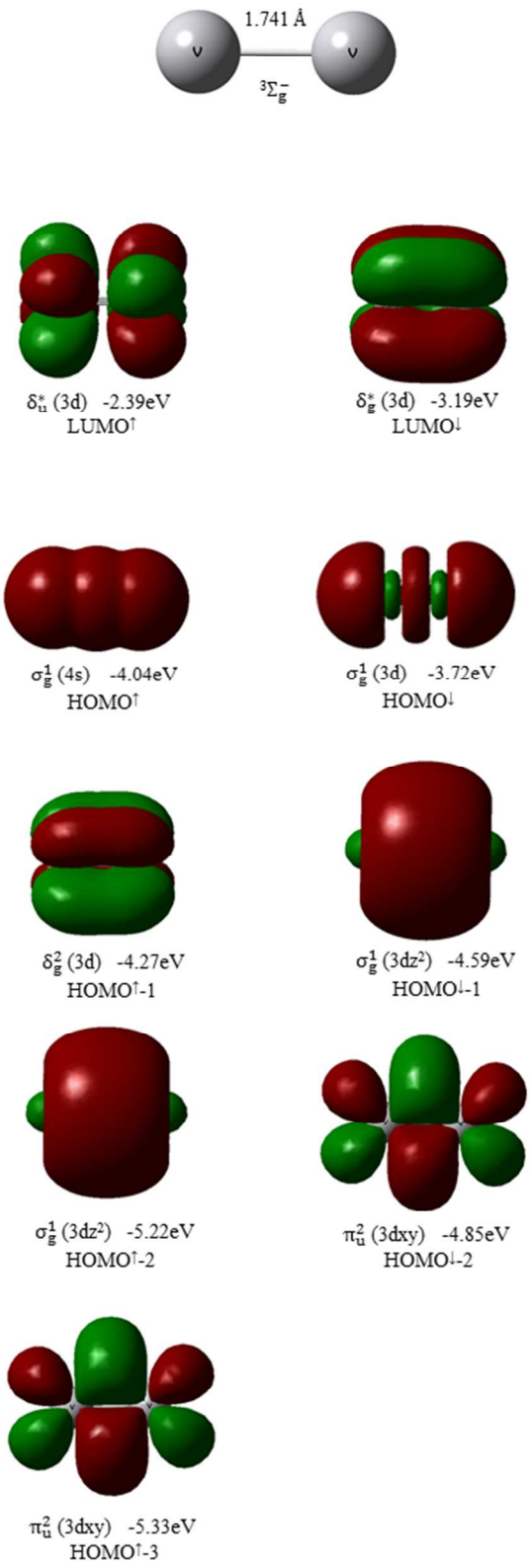

Figure S1. Frontier molecular orbitals for the lowest energy state of the V_2 dimer.

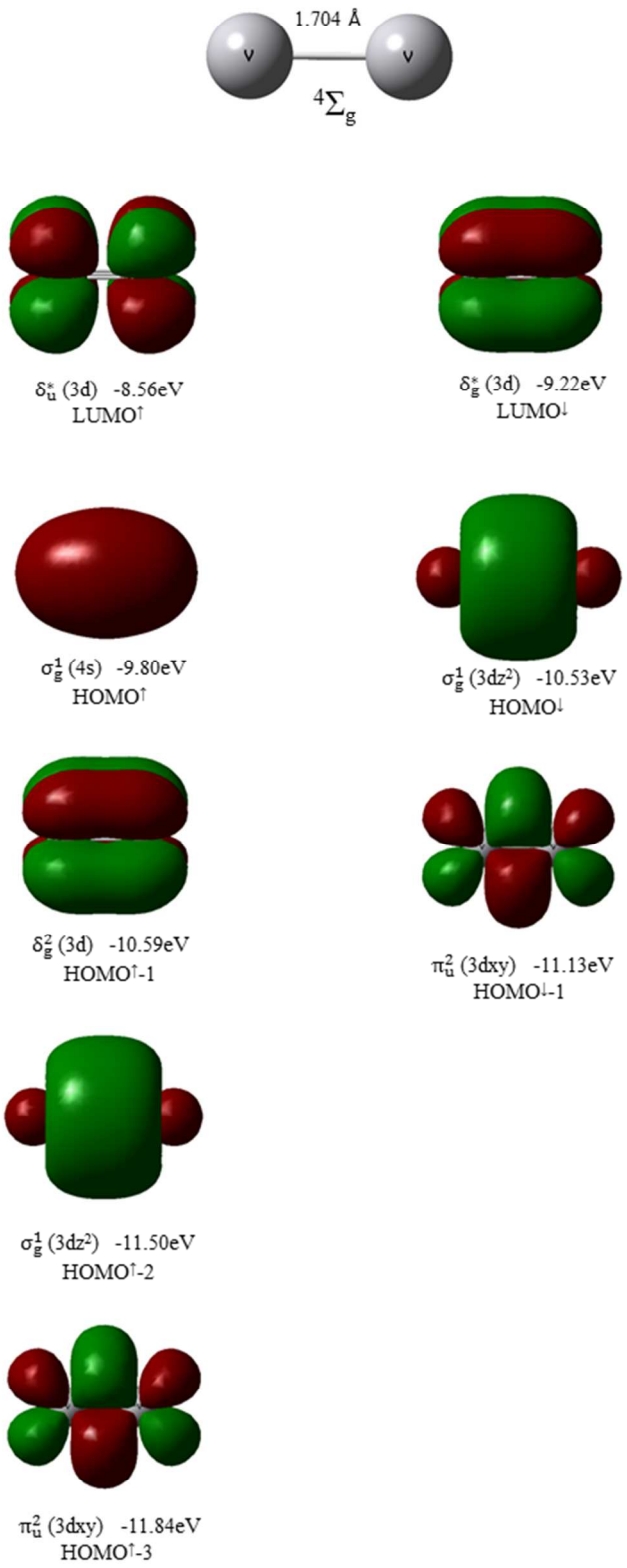

Figure S2. Frontier molecular orbitals for the ground state of the V_2^+ ion.

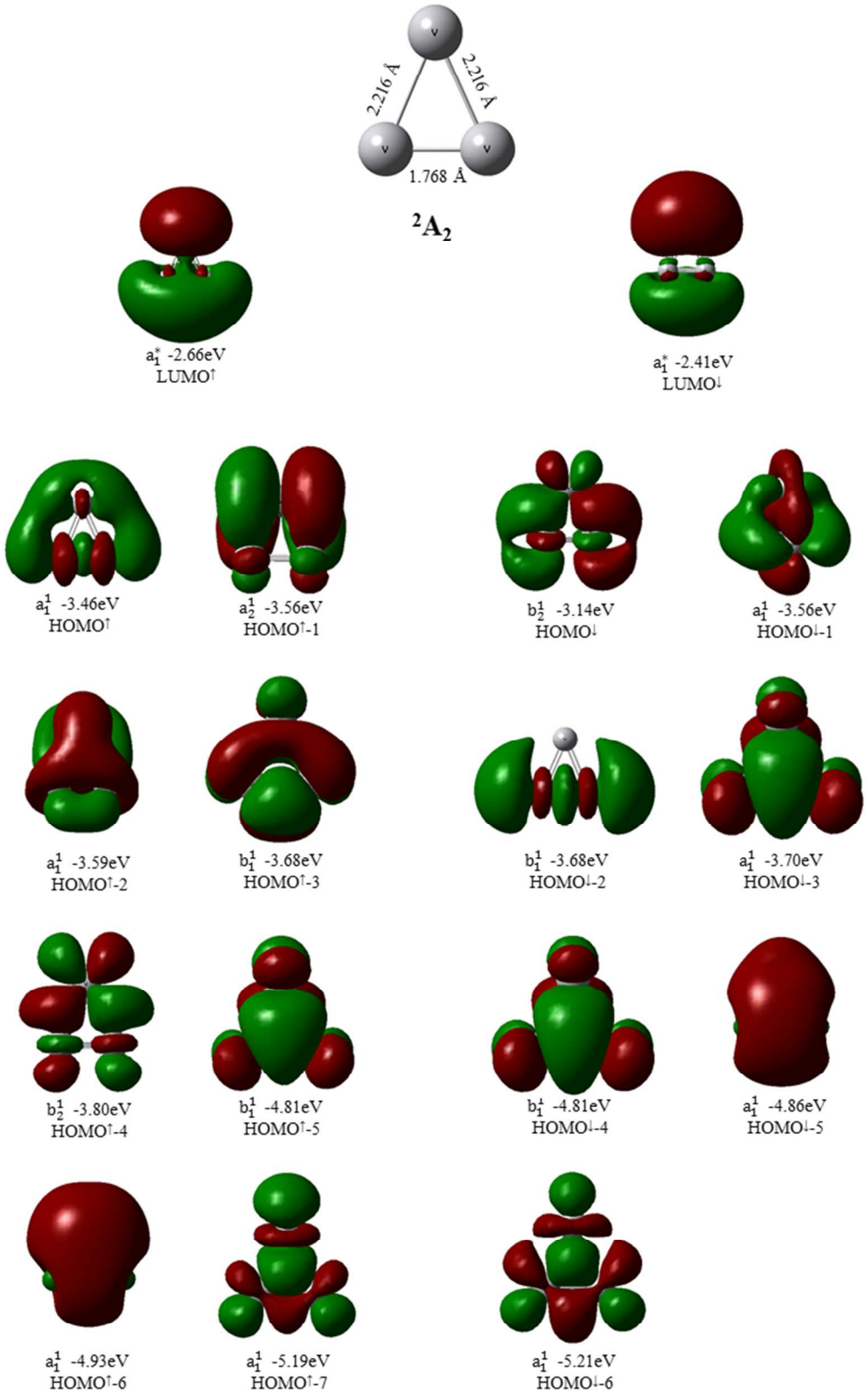

Figure S3. Molecular orbitals for the low-lying state of the V_3 cluster.

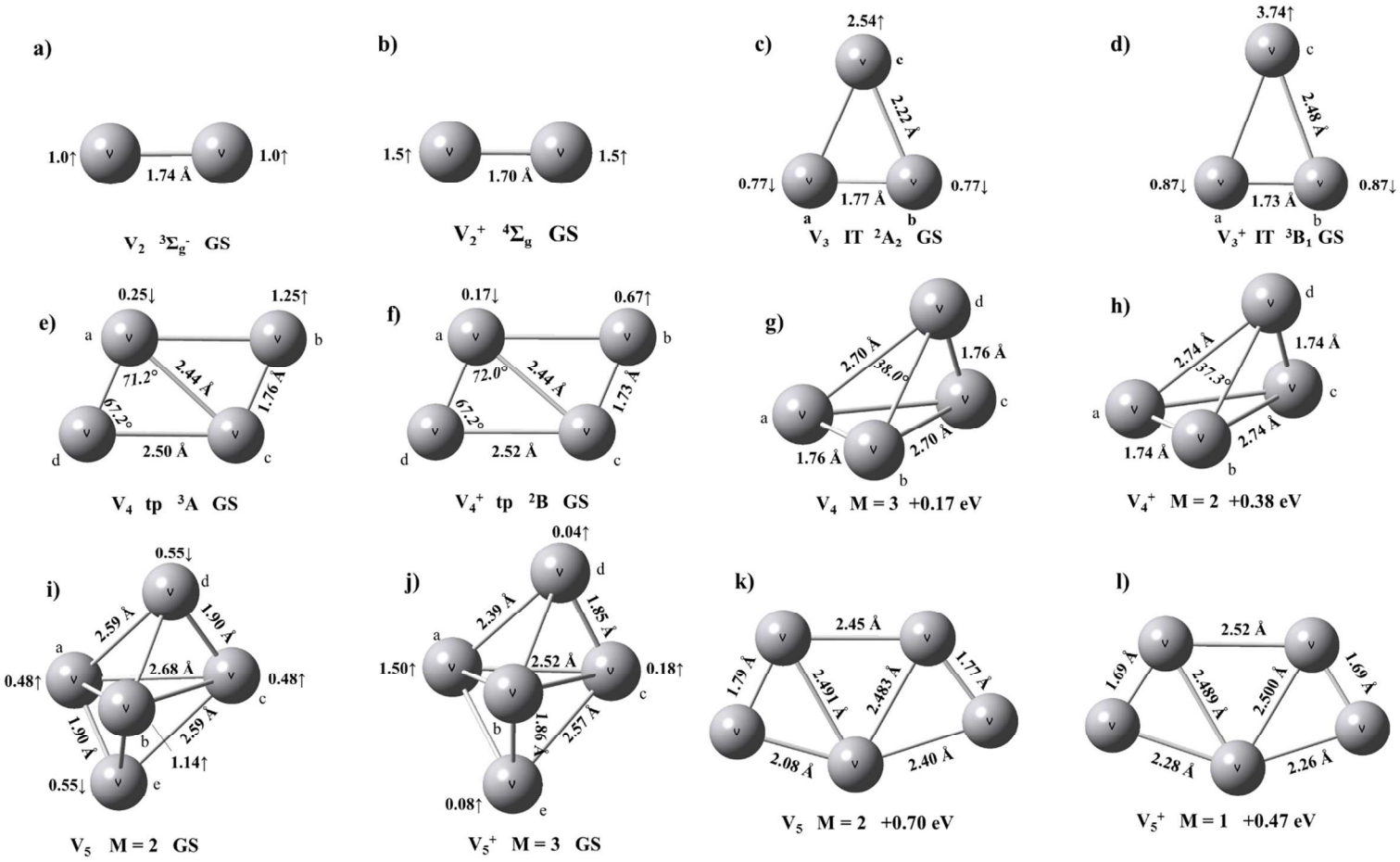

Figure S4. Calculated lowest energy structures for neutral and positively charged, $V_n^{0,+}$, $2 \leq n \leq 5$, clusters. Relative energies in eV, bond lengths in Å, NBO charges in electrons (e), and spin distributions (marked by arrows) are shown.

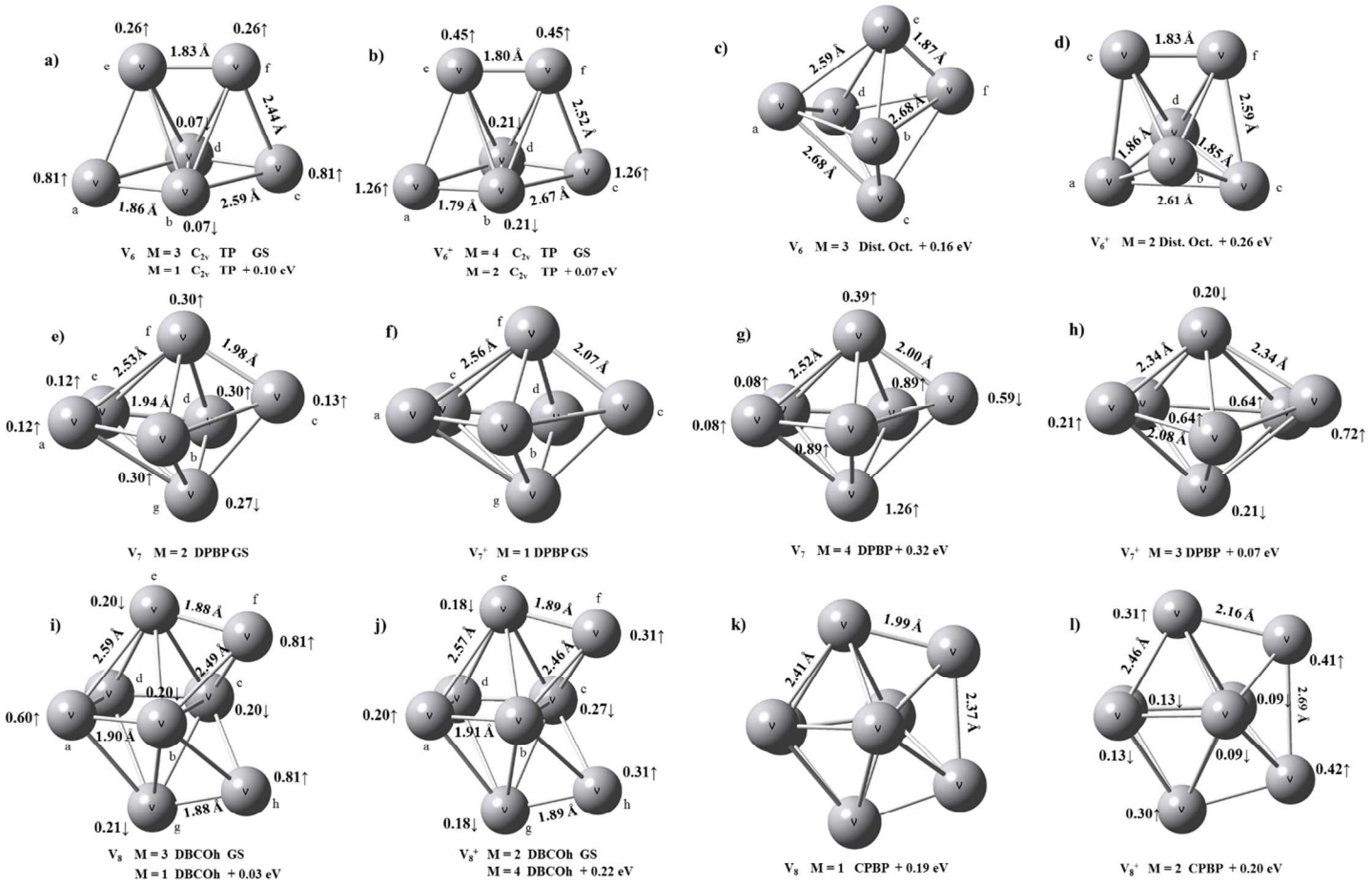

Figure S5. Lowest energy structures for neutral, V_n, and charged, V_n^+, $6 \leq n \leq 8$, clusters. Relative energies in eV, bond lengths in Å, charges in electrons (e), and spin distributions (marked by arrows) are shown.

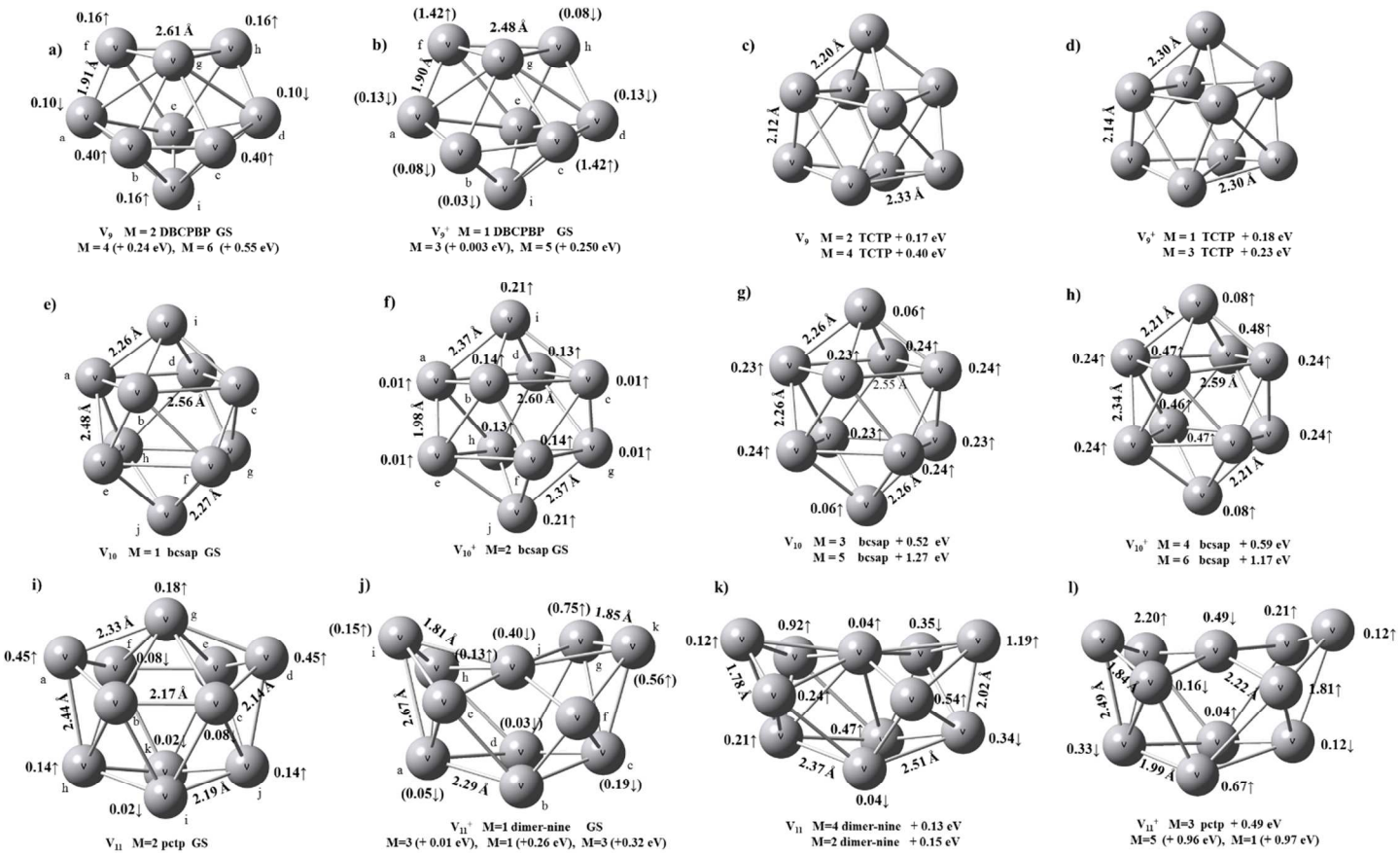

Figure S6. Most stable structures for neutral, V_n, and charged, V_n^+, $9 \leq n \leq 11$, clusters. Relative energies in eV, bond lengths in Å, charges in electrons (e), and spin distributions (marked by arrows) are shown.

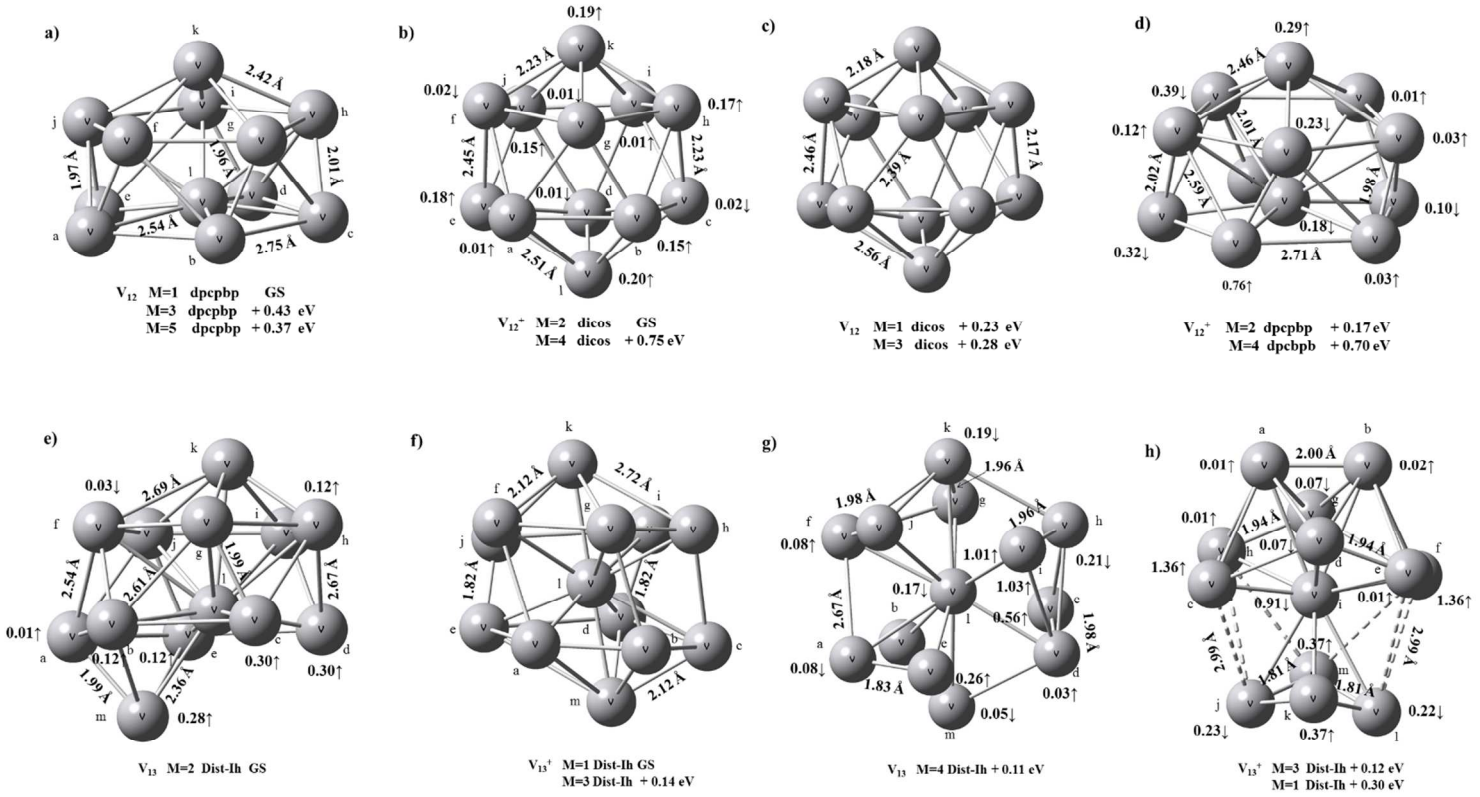

Figure S7. Lowest energy structures for neutral, V_n, and charged, V_n^+, $12 \leq n \leq 13$, clusters. Relative energies in eV, bond lengths in Å, charges in electrons (e), and spin distributions (marked by arrows) are indicated.

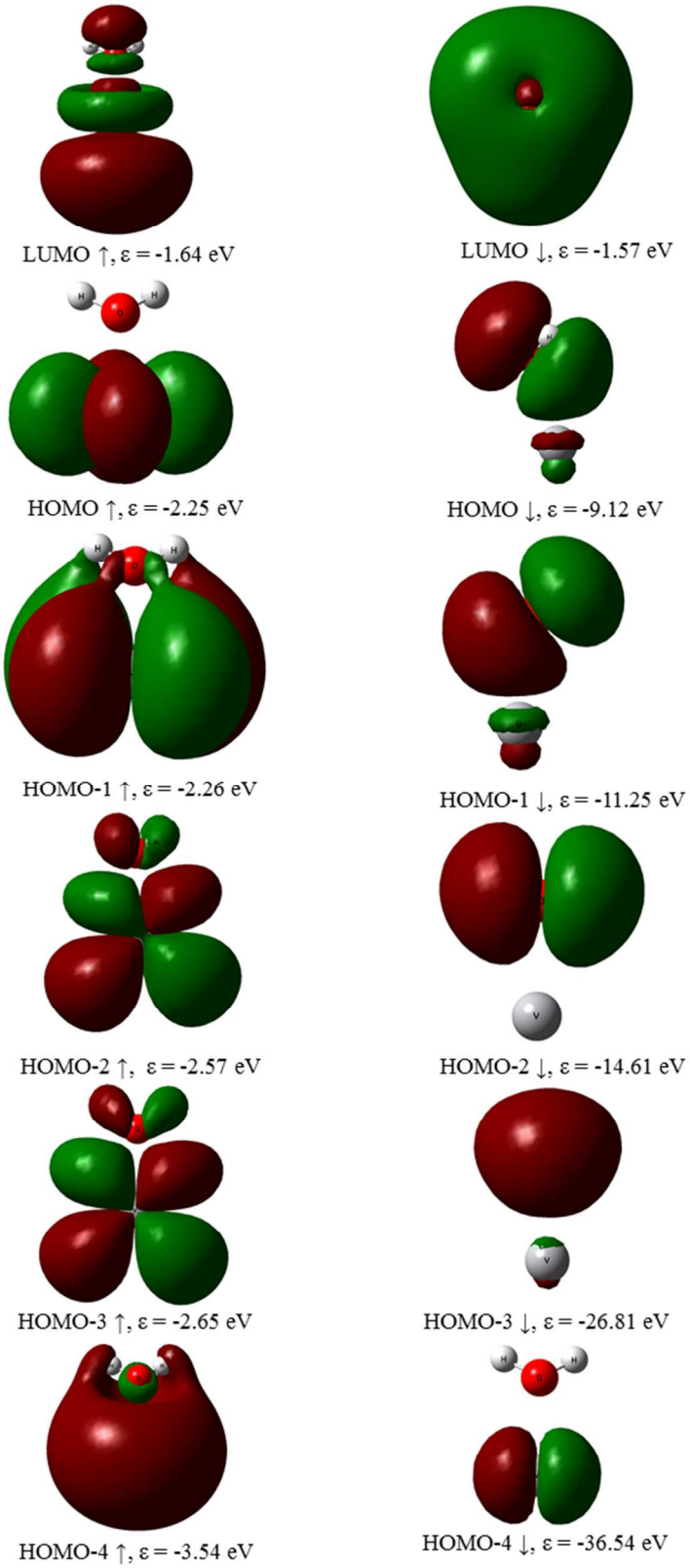

Figure S8. Frontier molecular orbitals for the low-lying state of the V–H_2O system.

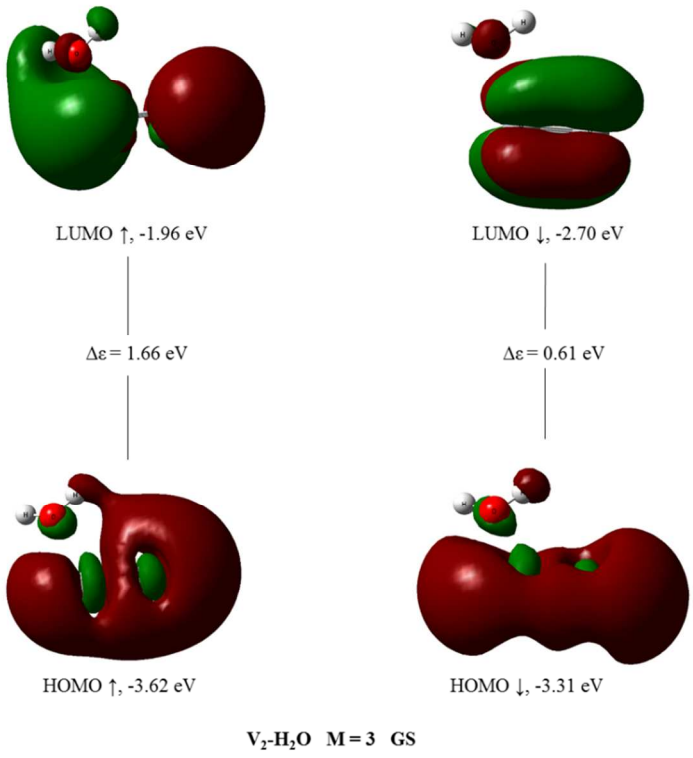

Figure S9. Contour plots for HOMO and LUMO of the V_2–H_2O cluster.

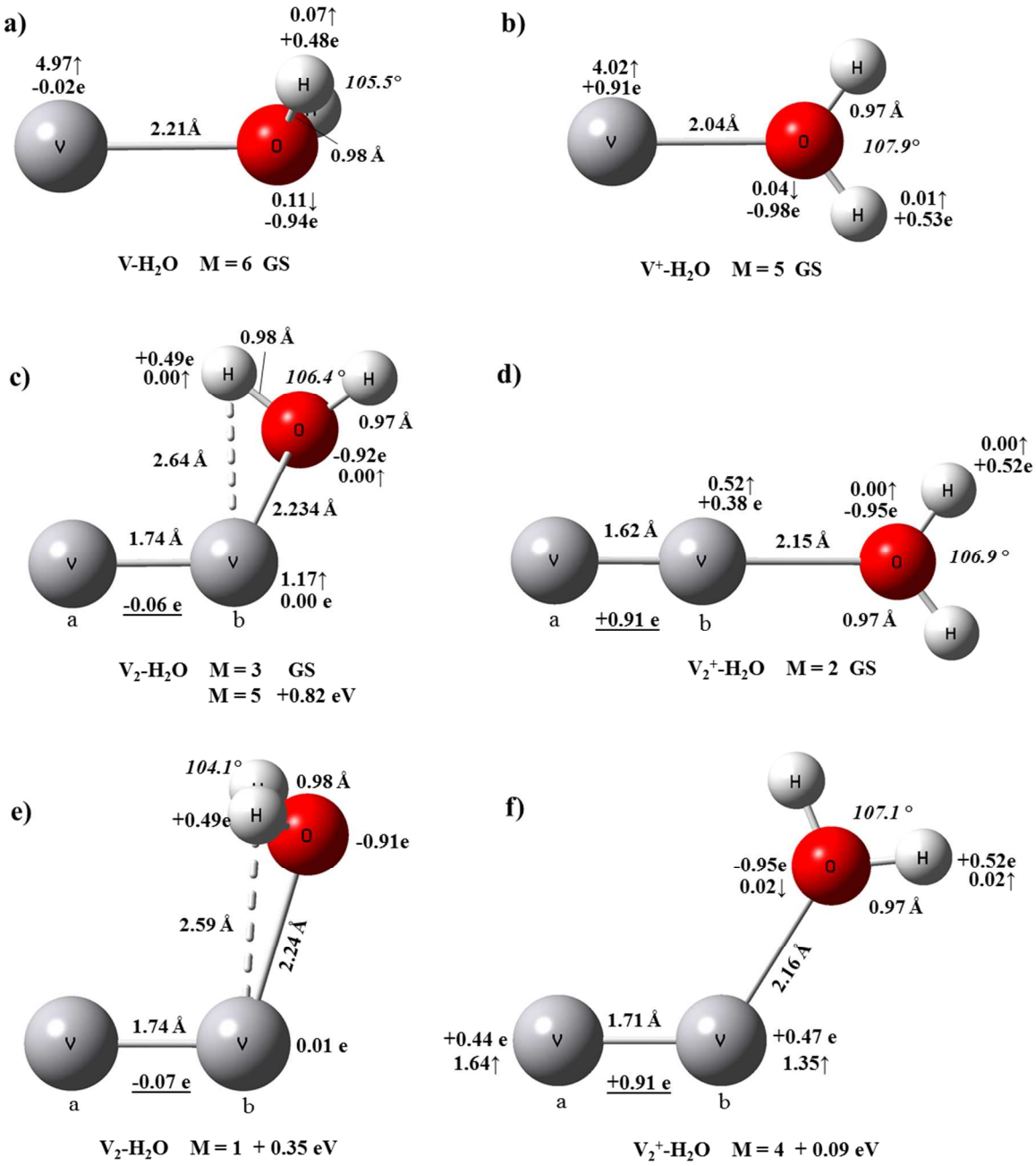

Figure S10. Lowest energy coordination modes for neutral, V_n-H_2O, and charged, V_n^+-H_2O, n = 1 and 2, systems. Relative energies, in eV, some distances, in Å, NBO charges in electrons (e), underlined values are for the total charge on the V_n subcluster, spin distributions (values with arrows) are indicated.

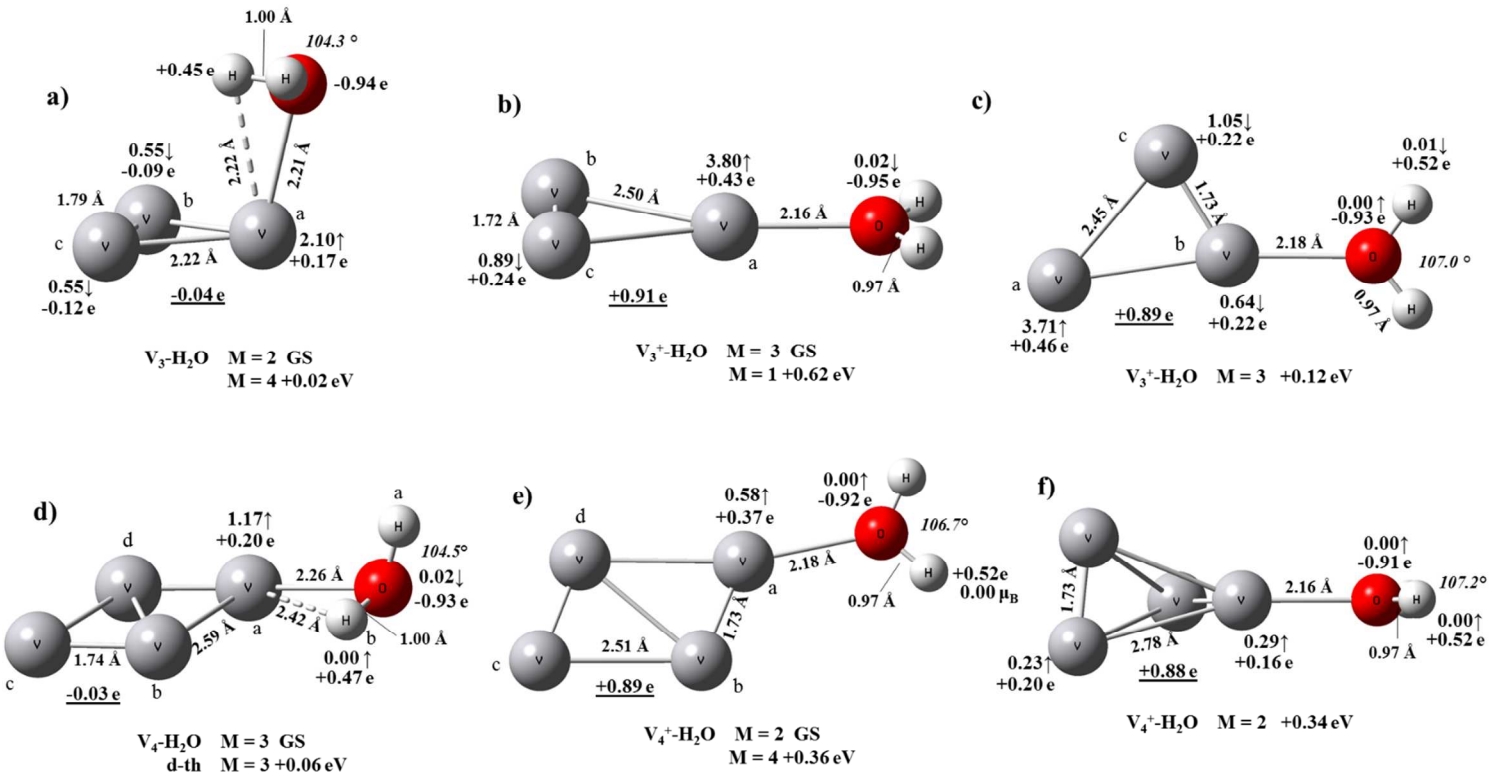

Figure S11. Lowest energy coordination modes for neutral, V_n-H_2O, and charged, V_n^+-H_2O, n = 3 and 4, clusters. Relative energies, in eV, some distances, in Å, NBO charges in electrons (e), underlined values are for the total charge on the V_n subcluster, spin distributions (marked by arrows) are indicated.

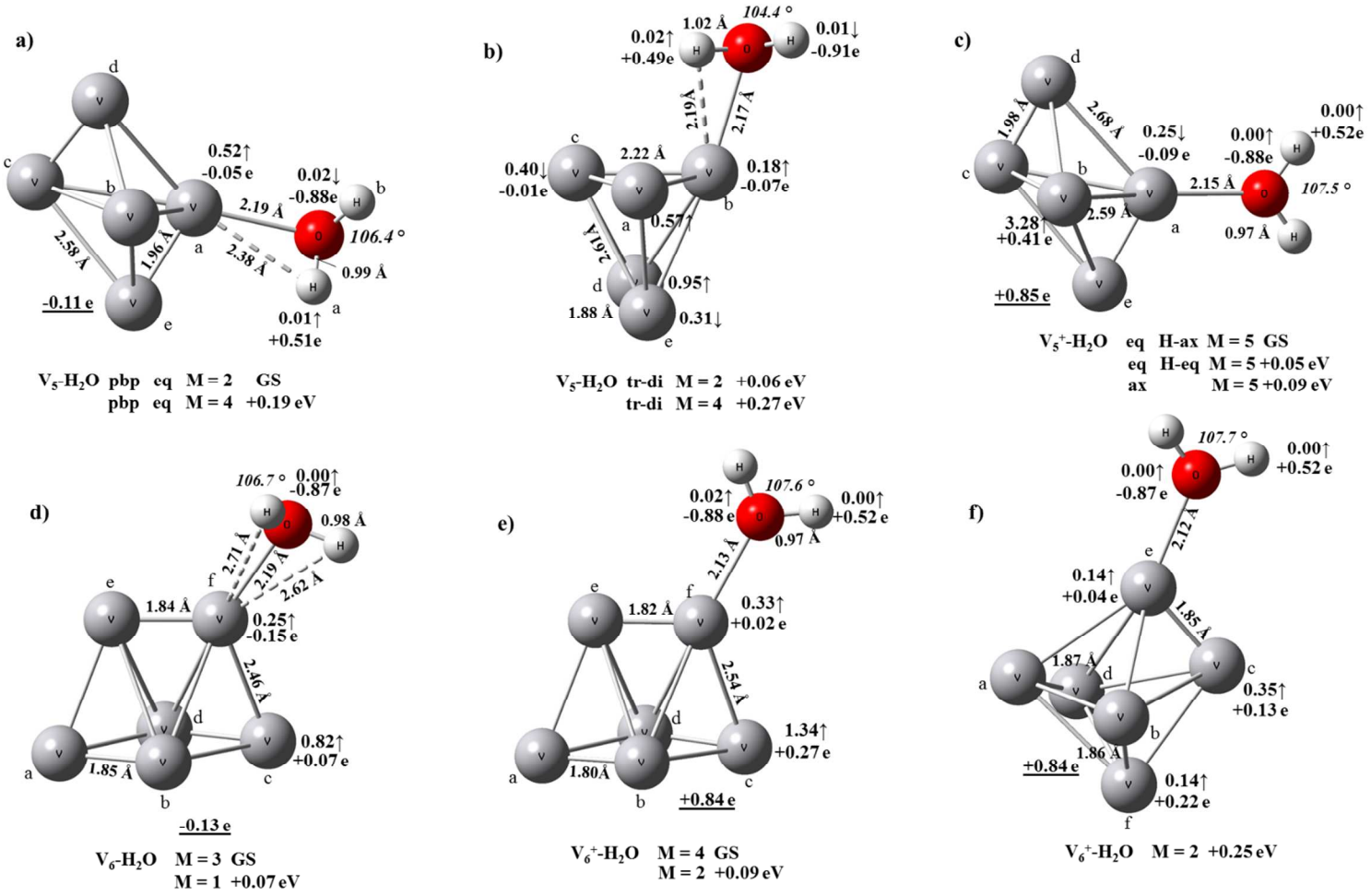

Figure S12. Lowest energy coordination modes for neutral, V_n-H_2O, and charged, V_n^+-H_2O, n = 5 and 6, clusters. Relative energies, in eV, some distances, in Å, NBO charges in electrons (e), underlined values are for the total charge on the V_n subcluster, spin distributions (marked by arrows) are indicated.

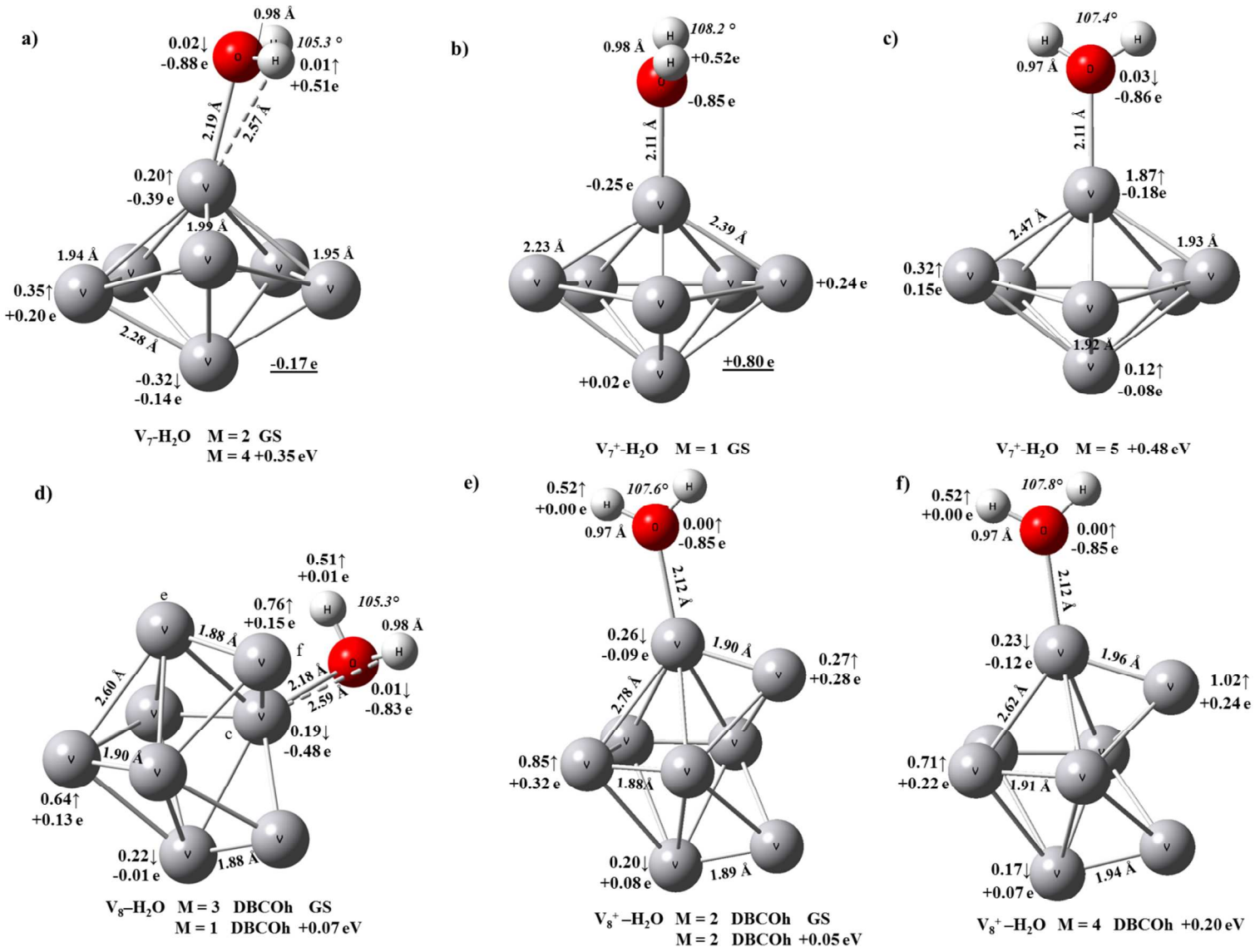

Figure S13. Lowest energy coordination modes for neutral, V_n-H_2O, and charged, V_n^+-H_2O, n = 7 and 8, clusters. Relative energies, in eV, some distances, in Å, NBO charges in electrons (e), underlined values are for the total charge on the V_n subcluster, spin distributions (marked by arrows) are indicated.

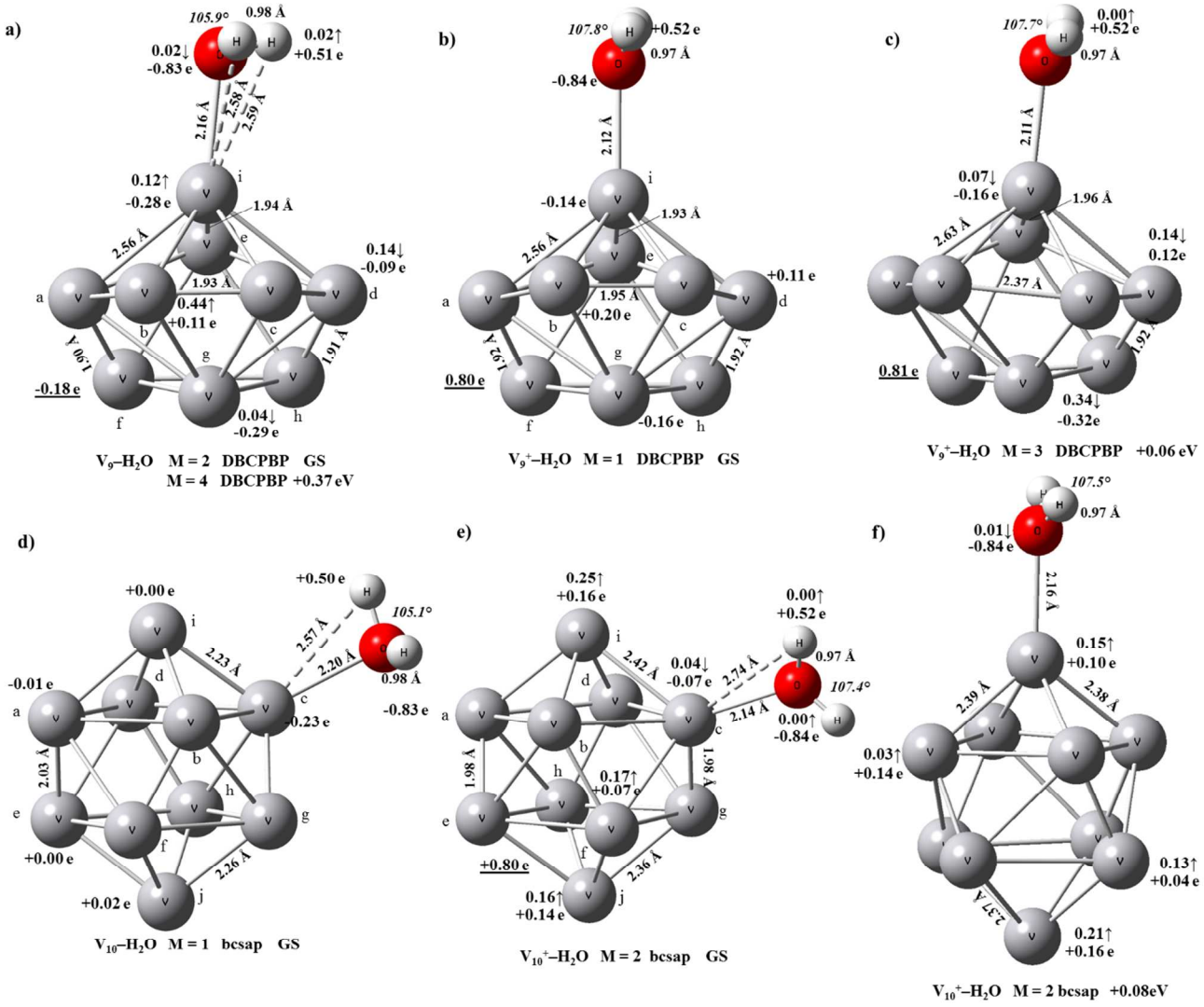

Figure S14. Lowest energy coordination modes for neutral, V_n-H_2O, and charged, V_n^+-H_2O, n = 9 and 10, clusters. Relative energies, in eV, some distances, in Å, NBO charges in electrons (e), underlined values are for the total charge on the V_n subcluster, spin distributions (marked by arrows) are indicated.

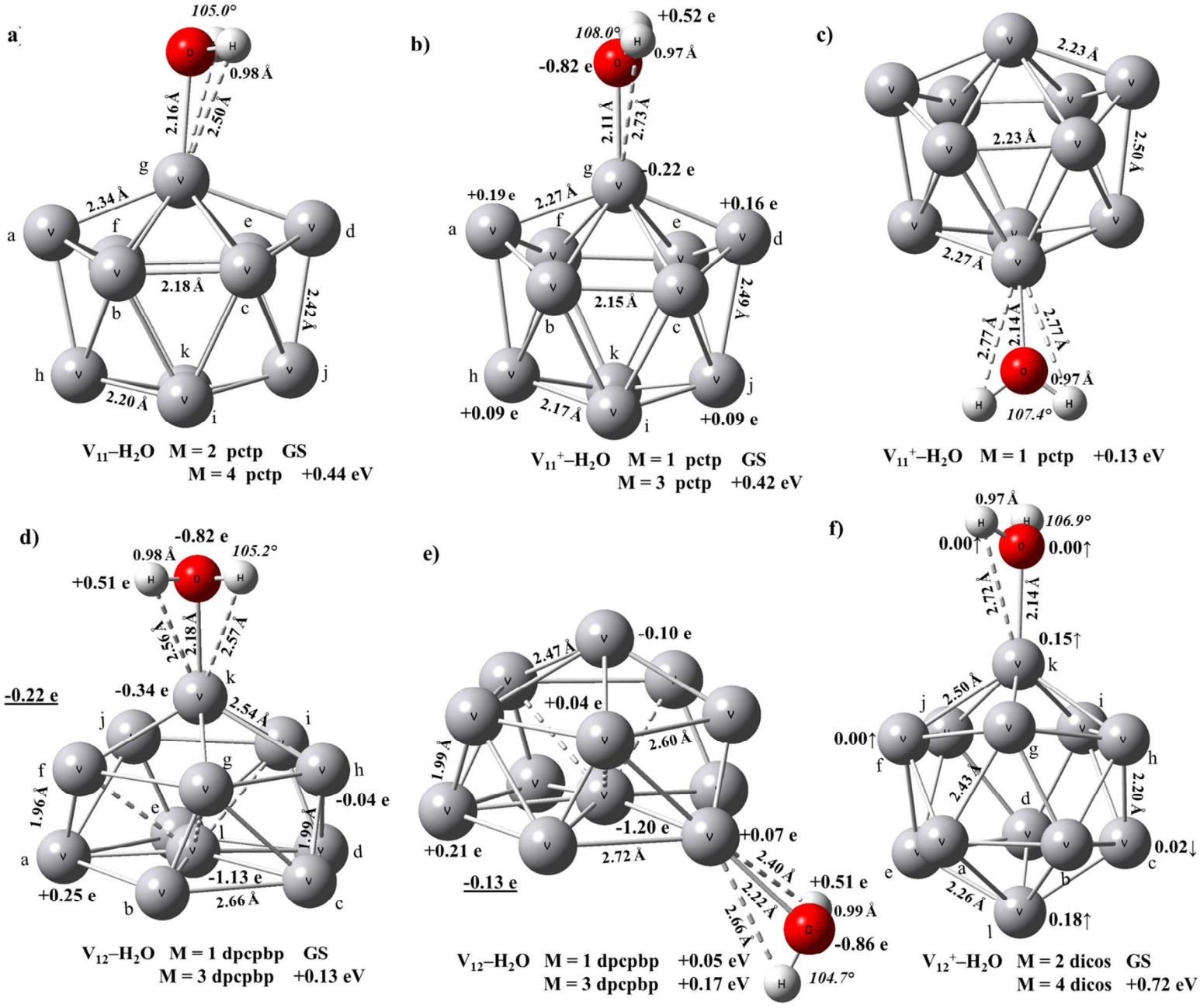

Figure S15. Lowest energy coordination modes for neutral, V_n-H_2O, and charged, V_n^+-H_2O, n = 11 and 12, clusters. Relative energies, in eV, some distances, in Å, NBO charges in electrons (e), underlined values are for the total charge on the V_n subcluster, spin distributions (marked by arrows) are indicated.

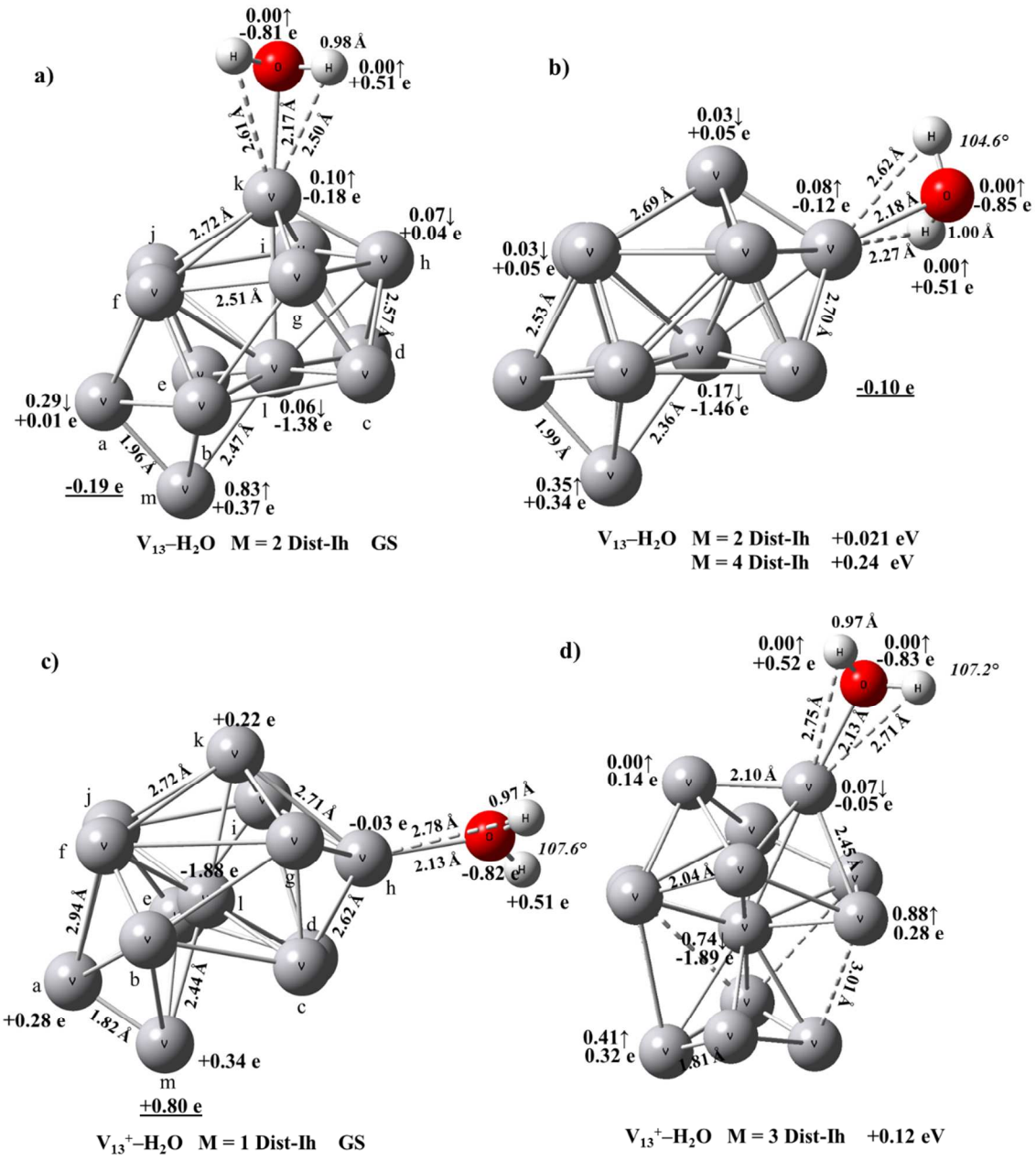

Figure S16. Lowest energy coordination modes for neutral, V_{13}-H_2O, and charged, V_{13}^{+}-H_2O, clusters. Relative energies, in eV, some distances, in Å, NBO charges in electrons (e), underlined values are for the total charge on the V_n subcluster, spin distributions (marked by arrows) are indicated.