THEORETICAL STUDIES OF THE VIBRATIONAL ENERGY LEVEL PATTERNS IN Ne_2SH AND Ne_2OH ($\tilde{A}\,^2\Sigma^+$)

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Variational calculations of the twenty-five lowest energy vibrational states of the Ne_2SH and Ne_2OH ($\tilde{A}\,^2\Sigma^+$) complexes are performed using potentials that are obtained by the pair-wise addition of accurate neon dimer and Ne·XH potentials (X = 0 or S). The Ne_2XH complexes are able to sample several local minima in their respective potentials at relatively low internal energies. Consequently, both complexes display average densities of states that exceed one vibrational state per cm^{-1} in the energy regime covered by this study. In spite of this, all of the calculated states are assigned to specific vibrational excitations, based on a structure of the complex that corresponds to one of the minima on the potential, and all of the minima are found to support progressions of bending states. In most cases, it is found that the wave functions have most of their amplitude in one of the potential minima, but the couplings between zero-order states that are localized in different minima increase as the internal energy is increased. The extent of mixing is found to depend on the symmetry of the wave functions with respect to the interchange of the two neon atoms. Effects of the differences in the anisotropies of the Ne·OH and Ne·SH potentials on the wave functions and vibronic spectra will also be discussed.