BOUND ROVIBRATIONAL ENERGY LEVELS FOR THE NeXH/D ($\tilde{X}^2\Pi, v_{XH} = 0, X = O, S$) VAN DER WAALS COMPLEXES

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Bound rovibrational energy levels for the complexes of a neon atom with OH or SH in their ground electronic state ($\tilde{X}^2\Pi$) are obtained by a variational calculation with $J = 3/2, 1/2$ using the potential energy surfaces recently developed by Cybulski and coworker.[a] In these calculations, a descrete variable representation (DVR) is employed for the intermolecular stretching coordinate and symmetrized Hund case (a) basis functions are used for the rotational motion of XH fragment. For both species, the ground states have linear geometries with the hydrogen atom pointing toward the rare gas atom. In the case of the SH complex, the motion of SH is found to be close to the free rotor limit, but the couplings induced by the potential and Coriolis terms in the Hamiltonian make the OH complex deviate significantly from the free rotor limit. A comparion with available experimental data is also made.

[a] S. M. Cybulski (to be published)