BOUND ROTATION–VIBRATION STATES FOR THE Ne_2XH ($\tilde{A}^2\Sigma, v_{HX} = 0$, X=O,S) VAN DER WAALS COMPLEXES

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The rotation–vibration states of Ne_2XH ($\tilde{A}^2\Sigma$) are obtained by variational calculations. The potential energy surfaces are described by a sum of the Ne–HX empirical potential surface developed by us[ab] and the Ne–Ne potential of Aziz.[c] In these calculations, the orthogonalized satellite coordinates are used in order to properly describe both the T–shaped and linear geometries of the complexes. The ground states of the Ne_2XH complexes are localized in the region of the potential that corresponds to the T–shaped geometry with the hydrogen atom pointing toward the center of mass of neon dimer. In the case of Ne_2OH, there are low lying states that are localized in the region of the potential that corresponds to the linear Ne–OH–Ne geometry. The complete rotation-vibration energy level progressions of Ne_2OH and Ne_2SH are presented. Comparisions with available experimental data and previous diffusion Monte Carlo results are also made.

[a] C. C. Carter, T. A. Miller, H. -S. Lee, A. B. McCoy and E. F. Hayes *J. Chem. Phys* **110**, 5065 (1999)
[b] H. -S. Lee, A. B. McCoy, L. B. Harding, C. C. Carter and T. A. Miller *J. Chem. Phys* **111**, 10053 (1999)
[c] R. A. Aziz and M. J. Slaman *Chem. Phys* **130**, 187 (1989)