EMPIRICAL POTENTIAL ENERGY SURFACE FOR THE $^2\Sigma$ STATE OF NeSH AND NeSD

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A semiempirical potential energy surface (PES) for the first excited state of the NeSH and NeSD van der Waals molecules will be presented. The potential energy functional form used in this study is the same as that proposed by Hutson for the NeHCl van der Waals complex.[a] The parameters in this functional form were modified using non-linear least square fitting to minimize the difference between the calculated and experimental energy levels and state-specific rotational constants. A detailed comparision between experimental measurements of Miller and coworkers [b] and the calculated values from optimized PES will be presented. The reliability of the spectral assignments, quality of the semiempirical surface and general features of the interaction potential will be discussed.

[a] J. M. Hutson, J. Chem. Phys. 91, 4448 (1989).

[b] C. C. Carter and T. A. Miller, private communication