A SEMIEMPIRICAL PES FOR Kr-HS

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A semiempirical potential energy surface for Kr-HS van der Waals type molecule will be presented. The nature of the PES is similar to that proposed for Ar-HO by Bowman and co-workers [1]. The parameters in the Ar-HO surface was modified using an efficient nonlinear fit program to agree with experimental measurements for Kr-HS molecule by Miller and co–workers [2]. The calculated results will be reported along with comparisons with the experimental results of Miller and co–workers. Quantitative insights into the interaction potentials for similar systems will be discussed.

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1. J. M. Bowman, B. Gazdy, P. Schafer, M. C. Heaven. J. Phys. Chem **94** 2226 (1990).
2. Private communication from T. A. Miller, Ohio State University.