DIATOM - DIATOM POTENTIAL ENERGY SURFACE FOR THE INTERACTION BETWEEN CN($A^2\Pi$) AND H_2

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There has been considerable recent interest in van der Waals complexes formed between open and closed shell diatoms. In the case of CN-H_2 spectra have been recorded for the $B^2\Sigma$-$X^2\Sigma$ and $A^2\Pi$-$X^2\Sigma$ transitions by Chen et al.[a] Previous calculations show that CN+H_2 in its electronic ground state has a collinear equilibrium structure[b] and there is barrier to the reaction H_2+CN$\longrightarrow$H+HCN proceeding via a linear transition state. Until now no similar information was available for the CN-H_2 in its electronic excited state. The purpose of our investigation was to generate an accurate Ab Initio potential energy surface for the CN($A^2\Pi$)+H_2 in the Van der Waals interaction region. A four-dimensional Ab Initio potential energy surface will be reported for the long-range interaction of H_2 with the open-shell CN diatomic in the its first electronic state $A^2\Pi$. The potential energy surface is based on a second order multireference perturbation calculation (CASPT2) utilizing a large correlation consistent basis set. The diatomic bond lengths were held constant in these calculations. The properties of the potential surface are compared with the spectrum reported earlier by Chen *et al.*[a] In addition, the potential energy surface is compared to recently reported *Ab Initio* calculations for H_2+O_2.

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[a] Y. Chen and M. C. Heaven *J. Chem. Phys.* **109**, 5171(1998).

[b] A. L. Kaledin, M. C. Heaven, and J. M. Bowman *J. Chem. Phys.* **110**, 10380(1999).