

## DIATOM - DIATOM POTENTIAL ENERGY SURFACE FOR THE INTERACTION BETWEEN CN(A<sup>2</sup>Π) AND H<sub>2</sub>

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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<sub>2</sub> spectra have been recorded for the B<sup>2</sup>Σ-X<sup>2</sup>Σ and A<sup>2</sup>Π-X<sup>2</sup>Σ transitions by Chen et al.<sup>a</sup> Previous calculations show that CN+H<sub>2</sub> in its electronic ground state has a collinear equilibrium structure<sup>b</sup> and there is barrier to the reaction H<sub>2</sub>+CN→H+HCN proceeding via a linear transition state. Until now no similar information was available for the CN-H<sub>2</sub> in its electronic excited state. The purpose of our investigation was to generate an accurate *Ab Initio* potential energy surface for the CN(A<sup>2</sup>Π)+H<sub>2</sub> 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<sub>2</sub> with the open-shell CN diatomic in its first electronic state A<sup>2</sup>Π. 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.*<sup>a</sup> In addition, the potential energy surface is compared to recently reported *Ab Initio* calculations for H<sub>2</sub>+O<sub>2</sub>.

<sup>a</sup>Y. Chen and M. C. Heaven *J. Chem. Phys.* **109**, 5171(1998).

<sup>b</sup>A. L. Kaledin, M. C. Heaven, and J. M. Bowman *J. Chem. Phys.* **110**, 10380(1999).