Study of the CN($^2\Sigma$) + N(^{4}S) reaction at high temperatures

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The CN molecule plays an important role in the chemistry around the surface of a spacecraft during the atmospheric re-entry. The collision of CN with others molecules and atoms has a particular interest in aerothermodynamic modeling.[1] This work focuses on studying the CN+N ↔ N_2+C reaction within the triplet manifold 3A" of CN_2. Recent theoretical studies have explored this reaction[2]. However, the number of analytical potential energy surfaces (PES) is reduced, and computed at the CASPT3 level[3] or limited to a two-dimensional surface[4]. Here, we developed a full dimensional high-level PES for this system from *ab initio* calculations at the MRCI-F12 level of theory. Then this new surface is used in quasi-classical trajectory calculations. Thermal rate coefficients are computed from 100 to 20000 K. The computed rates for the CN+N → N_2+C reaction are compared with available experimental data, and a good agreement is found. At low and intermediate temperatures, the N_2 formation is more efficient than the N-exchange, while at high temperatures, the rates for both channels are comparable. Finally, analytical modified Arrhenius expressions of the rates for the N_2 formation and N-exchange reactions are reported.

References

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