Energetics and Kinetics of Various Cyano Radical Hydrogen Abstractions

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The cyano radical (CN) is an abundant, open-shell molecule found in a variety of environments, including the interstellar medium and combustion processes. In these environments, it often reacts with small, closed-shell molecules via hydrogen abstraction. Both carbon and nitrogen are reactive sites, however the carbon is more reactive with reaction barrier heights generally between 2 – 13 kcal mol^{-1} lower than those of the nitrogen. The CN + HX $\rightarrow$ HCN/HNC + X, where X = H, CH_3, NH_2, OH, C_2H, Cl, Br, F, CN, PH_2, SH, HCO, NCO, CH_3O, CH_2OH, reactions have been studied at a high-level of theory, including CCSD(T)-F12. Diagonal Born-Oppenheimer and relativistic effects were also determined and contribute to the reaction enthalpies. Additionally, accurate kinetics were obtained at a wide range of temperatures (20 – 5000K) which are in excellent agreement with existing experimentally determined rate constants.