Elementary reactions of O(^{3}P), N(^{2}D), and CN radicals of relevance in astrochemistry: Combined crossed-beams and theoretical studies

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Oxygen, carbon, and nitrogen are the 3rd, 4th and 5th most abundant elements in the interstellar medium (ISM). N_2 is by far the main constituent of the tick atmosphere of Titan where, in its upper part, it readily produces excited N(^{2}D) atoms, which are known to play an important role being very reactive with all present molecules, such as saturated (CH_4) and unsaturated (alkynes, alkenes) hydrocarbons as well as aromatics (C_6H_6), and nitriles (such as HCCCN, CH_2CHCN). Also CN radicals, which are ubiquitous and largely abundant in the ISM, are readily formed in Titan's atmosphere. The above two nitriles (cyanoacetylene, vinylcyanide) are also present in the ISM. Hence, reactions of N(^{2}D) with species as propyne, allene, and benzene, and of N(^{2}D), CN, and also O(^{3}P) with HCCCN and CH_2CHCN are relevant in Titan's atmosphere, the ISM, and also combustion. Over the past several years we have been investigating, under single-collision conditions, a large variety of bimolecular reactions involving the above radicals using the crossed molecular beams (CMB) technique with mass spectrometric detection, combined to electronic structure calculations of the potential energy surfaces and related statistical calculations of product branching fractions (BFs), including intersystem crossing when present.[1-9] The goal has been to unravel the reaction dynamics and provide useful information for improved kinetic models of those exotic environments. In fact, once the theoretical results are found validated by a satisfactory comparison with experimental results in CMB conditions, the theoretical approach is used to predict product BFs and, often, also *channel-specific rate constants* as a function of temperature *T* (from low to high *T*), which are the needed information for improving current kinetics/photochemical models of the ISM and of Titan's atmosphere, as well as of combustion environments.

In this talk, we will discuss the results of some of our recent, synergistic experimental and theoretical studies on reactions of O(^{3}P) and N(^{2}D) with aliphatic and aromatic hydrocarbons, including pyridine (one of the simplest aromatic heterocyclic molecules) and nitriles, and also on reactions of CN with nitriles, all of astrochemical relevance.[1-9] The implications for improved photochemical models of the ISM and Titan's atmosphere will be commented on.

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