A Novel Instrument to Study the Cosmic Origins of Organic Chemistry

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Abstract

We propose to recreate, in a highly controlled manner, the most fundamental steps of interstellar chemistry that initiate not only the formation of organic molecules in the cosmos, but also provide some of the first threads in the knitting together of atoms and molecules into solid material. These processes are critical for the eventual formation of planets and likely also determine a major component of the organic chemistry that is present on their young surfaces. In specific, we will focus on reaction studies of neutral atomic carbon with molecular ions which are believed to initiate interstellar organic chemistry. Our understanding of these reactions is limited. Previous laboratory work has been difficult to interpret due to the challenge of producing and characterizing atomic C beams. Theory has been limited to highly uncertain classical methods as fully quantum mechanical reactions for systems with four or more atoms are beyond current computational capabilities.

We propose to develop a unique instrument which will not suffer from the limitations of previous experimental methods. We will use laser photodetachment of a C^- beam to generate a C beam. The C^- will then be removed electrostaticly leaving a pure C beam. We will next merge a molecular ion beam with the C beam so they are co-propagating. Using beams at keV lab energies will allow for ease of handling and characterization. Because the beams are co-propagating, we will be able to investigate reactions down to collision energies corresponding to molecular cloud temperatures. Reaction channels will be studied using a charge-to-mass analyzer to separate and detect the charged end products. Measuring all the relevant currents, beam shapes, energies, signal counts, and background rates will allow us to determine absolute cross sections for both reactions.

Our proposed astrobiology technology development is urgently needed for interpreting the molecular cloud spectra which will be collected in the coming decade. However, a source of funding for this project remains to be found. The level of support required exceeds by a factor of ~ 6 the average grant awarded by programs which have traditionally supported laboratory astrophysics such as the NASA Astronomy and Physics Research and Analysis (APRA) program and the NSF Astronomy and Astrophysics Grants (AAG) program. Our proposed astrobiology research also falls outside the mandate or funding history for those NASA and NSF programs which could potentially provide support at the level required for the proposed instrument development. The NASA Astrobiology Science and Technology Instrument Development (ASTID) program is for satellites, payloads, and flight hardware. The NSF Division of Astronomical Sciences Advanced Technologies and Instrumentation (ATI) program has historically supported only development of equipment and detectors which can be attached to telescopes. Neither program has funded laboratory astrophysics; and, not surprisingly, our proposal has been declined by each program. Progress in this critically needed area of astrobiology will come about only with a targeted investment in the development of our proposed ground breaking technology in laboratory astrophysics.

1. Introduction

The cosmic pathway towards life is thought to begin in molecular clouds when atomic carbon is “fixed” into molecules (Herbst 1995). These reactions initiated the formation of organic molecules, and also provided some of the first threads knitting atoms and molecules into solid material. Such processes are critical for the eventual formation of planets and may determine a major component of the organic chemistry present on their young surfaces.

Here we propose to develop and construct a unique instrument to study these first links in the chain of carbon chemistry leading towards life. Our innovative apparatus will provide important laboratory data to more deeply understand molecular cloud chemistry, thereby enabling more reliable interpretations of molecular cloud spectra. We will apply the new hardware and technology to astronomical research by selecting those chemical reactions predicted to be most important for understanding the cosmic origins of organic chemistry.

This white paper is organized as follows: In the rest of this section we discuss the astrophysical motivation and importance of our proposed advanced technology and instrumentation development. Section 2 briefly reviews previous experimental and theoretical chemical studies with neutral atomic carbon (hereafter, C). In §3 we describe our proposed research, the advanced technology that we will develop, the feasibility, and the advantages over past methods. Required resources are outlined in §4 and the reason a targeted investment is needed is described in §5. Lastly milestones are presented in §6.

1.1 Towards an Understanding of the Molecular Universe

Observations of molecular lines are used extensively to understand the molecular universe and its role in the chemical pathway towards life. To this end, a wide array of ground-based, airborne, and space-based observatories have been built or are being built.

Interpreting spectral observations from these observatories requires the use of sophisticated astrochemical models (Wakelam et al. 2006a; Woodall et al. 2007). Such models are utilized extensively throughout astronomy and have been used to interpret spectra from diffuse and dark interstellar clouds (Belloche et al. 2002; Lee et al. 2004; Neufeld et al. 2006; Snow & McCall 2006), photon-dominated regions (PDRs; Neufeld et al. 2005; Le Petit et al. 2006), interstellar shocks (Tielens 2005), young stellar objects (YSOs; Lahuis & van Dishoeck 2000; Charnley et al. 2001; Schöier et al. 2002; Doty et al. 2004), circumstellar envelopes (Brown & Millar 2003; Willacy 2004; Hasegawa et al. 2006; González-Alfonso et al. 2007), protoplanetary disks (Ilgner et al. 2004; Semenov et al. 2005; Vasyunin et al. 2008), protoplanetary nebulae (Herpin et al. 2002; Cernicharo 2004; Woods et al. 2005), and hot molecular cores (Snell et al. 2000; Molinari et al. 2002; Nomura & Millar 2004).

However, our chemical understanding of the universe is limited by uncertainties in the reaction data used in astrochemical models. These uncertainties are due to a combination of a) limitations in current experimental techniques which often have large uncertainties, b) limitations in current experimental capabilities worldwide making it impossible to measure rate coefficients for many of these systems, and c) the complexity of molecules with many degrees of freedom making quantum calculations computationally prohibitive.

The most sophisticated models include 4500+ gas-phase reactions and about 450 atomic and molecular species. Measurements are lacking for well over half of these and the adopted rate coefficients used for these unmeasured reactions are estimated to have at least a factor of 2 uncertainty (Woodall et al. 2007; Vasyunin et al. 2008; see also §2.).

Identifying the key reactions whose uncertainties most limit the reliability of the models has become an area of intense interest (Wiebe et al. 2003; Vasyunin et al. 2004; Wakelam et al. 2005, 2006a,b; Vasyunin et al. 2008). This helps researchers to focus their efforts in experimental and theoretical molecular studies to better address the needs of the astrophysics community. For example, Vasyunin et al. (2008) studied how uncertainties in these 4500+ reactions affect the abundances and column densities for 15 key species in protoplanetary disks. These commonly observed species include CO, C^+, H_3^+, H_2O, NH_3, N_2H^+, $HCNH^+$, CS, CO_2, HCO^+, H_2CO, C_2H, CN, HCN, and HNC. Vasyunin et al. identified 56 reactions whose rate coefficients need to be determined more accurately into order to improve the reliability of current astrochemical models for these 15 key species. Nine of these reactions involve atomic C. The work we propose here will help to remove the uncertainties for several of these key reaction involving C (see §1.3).

1.2 Carbon in Molecular Clouds

The known chemistry in space is largely carbon based. Over 150 interstellar and circumstellar molecular species have been identified in the gas-phase. Of these 113 are carbon bearing and slightly over half of the known gas-phase molecules are organic in nature (http://www.astrochemistry.net).

Atomic C has been observed in molecular clouds such as MCLD 123.5+24.9 (Bensch et al. 2003), AFGL 333 (Sakai et al. 2006), W3 (Sakai et al. 2006), Barnard 68 (Pineda & Bensch 2007), and the Carina region (Kramer et al. 2008). Atomic C plays a critical role in the initial reactions of organic chemistry in molecular clouds (see §1.3). Models indicate that atomic C is the dominant form of carbon from $\sim 10^3 - 10^5$ yr (van Dishoeck 1998). These times are comparable to the age of many observed molecular clouds (Herbst & Millar, in press).

The gas-phase chemistry of molecular clouds is constrained by the low temperatures and low densities of the clouds (Herbst 1995; van Dishoeck 1998; Herbst & Millar, in press). Because of the low densities, three-body processes are unimportant. Hence, for the gas-phase chemistry, one needs only consider two-body reactions. Low temperatures rule out ordinary neutral-neutral chemical reactions, which generally possess significant activation energies. For this reason ion-neutral reactions, which typically possess no activation barrier, are extremely important in astrochemistry (Woodall et al. 2006).

We add that it is also critical to accurately understand gas-phase two-body reactions in order to determine the importance of surface chemistry on dust grains. Astronomical observations can be used to infer molecular abundances. These results can then be compared to models of gas-phase interstellar chemistry allowing us to determine if the inferred chemical abundance for a given observed molecule can be explained solely by gas-phase chemistry. If not, then that implies that surface reactions on dust grains are important for that molecule. Given the greater complexities and unknowns of grain surface chemistry compared to gas-phase, such knowledge is likely to be the most direct approach to better understanding interstellar gas-grain chemistry.

1.3 The Beginnings of Organic Chemistry in Molecular Clouds

The initial steps in the carbon chemistry of molecular clouds begin with reactions involving C and C^+. For our proof-of-principle measurement, we propose to study the reaction

$$C + H_3^+ \;\rightarrow\; CH^+ + H_2, \tag{1}$$

H_3^+ is ubiquitous in both diffuse and dense molecular clouds (Geballe 2006; McCall 2006),

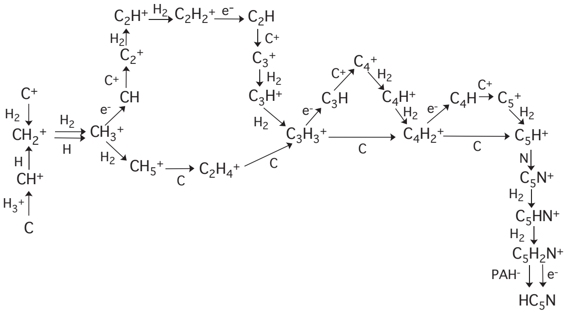

Figure 1: Chemical network for the formation of HC_5N showing two competing pathways. Determining the relative importance of each depends in part on accurate rate coefficients for reactions of atomic C with various molecular ions such as H_3^+, CH_5^+, $C_2H_4^+$, $C_3H_3^+$, and $C_4H_2^+$ (Wakelam & Herbst 2008; Wakelam 2008).

thereby making reaction 1 one of the first steps towards organic chemistry in molecular clouds (e.g., Van Dishoeck 1998; Herbst & Millar, in press).

Vasyunin et al. (2008) have identified reaction 1 as one of their 56 key reactions. They estimate there is a factor of 2 uncertainty in the recommended rate coefficient. Another reaction they identify as being important for models of protoplanetary disk chemistry is

$$\mathrm{C} + \mathrm{HCO}^+ \rightarrow \mathrm{CO} + \mathrm{CH}^+. \tag{2}$$

Atomic C is also important in the formation of complex hydrocarbons (see Fig. 1; Wakelam & Herbst 2008; Herbst & Millar, in press). This can occur via reactions such as

$$\mathrm{C} + \mathrm{C}_m\mathrm{H}_n^+ \rightarrow \mathrm{C}_{m+1}\mathrm{H}_{n-x}^+ + \mathrm{H}_x. \tag{3}$$

Experimental data are lacking for both reactions 2 and 3 and the uncertainties in the rate coefficients are estimated to be a factor of 2 (Woodall et al. 2007; Herbst & Millar, in press).

2. Previous Studies of Atomic C Chemistry

Completely quantum mechanical calculations for tetra-atomic or more complicated systems are beyond current theoretical capabilities (Bettens & Collins 1998). As a result, for reactions involving C with molecular ions the theoretical data used are all variants of classical trajectory theory (Prasad & Huntress 1980; Woodall et al. 2007). The uncertainties in such calculations are commonly at a factor of 2 or more (see Fig. 2).

Measurements of reaction cross sections and rate coefficients with atomic C have been severely limited due to the high reactivity of carbon and the resulting challenge of preparing a controlled, intense, and well characterized C beam (Kaiser & Suits 1995; Savić et al. 2005). To the best of our knowledge there are only two such published experimental studies.

The Gentry group neutralized a beam of C^+ by passing it through a gas cell where the ions could capture an electron. In this way they studied (Schutte & Gentry 1983)

$$\mathrm{C} + \mathrm{D}_2^+ \rightarrow \mathrm{CD}^+ + \mathrm{D}. \tag{4}$$

However, a major limitation of the electron capture method is the production of unknown fractions of metastable C atoms. Thus when studying reactions with ground term C, Schutte & Gentry were forced to divide the measured signal rate by the total C density (instead of the smaller unknown ground term density), thereby yielding only a lower limit to the resulting cross section. Additional complications due to the metastable C arise from the internal excitation energies of $\gtrsim 9,800$ K which could potentially alter the chemistry being studied.

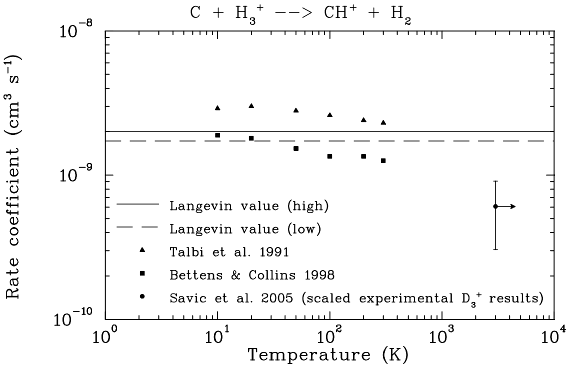

Figure 2: Rate coefficients for the reaction 1 showing the Langevin results (using the range of published polarizibilities for C from Nesbet 1977) and the classical trajectory theoretical results of Talbi et al. (1991) and Bettens & Collins (1998). The experimental result from Savić et al. (2005) on D_3^+ has been scaled by the reduced masses of the C/H_3^+ and C/D_3^+ systems.

The Gerlich group generated an effusive carbon beam using high temperature vaporization of carbon rods (> 3000 K) and directed the beam at ions stored in a trap (Savić et al. 2005). They studied the fully deuterated form of reaction 1. Their results differ from classical theory by a factor of ~ 5 (see Fig. 2). There are several limitations to the vaporized graphite approach: (1) The beam is not pure and the C_n ($n \geq 2$) impurities can react with the trapped ions complicating the data analysis; (2) The carbon source emits vacuum ultraviolet (VUV) radiation which can cause ionization in the trap and alter the chemistry occurring; (3) Trapped ionic end products can undergo subsequent parasitic reactions with either parent ions or background gas, complicating the interpretation and analysis of the data; (4) The carbon beam is emitted in bursts and has an unknown density which varies spatially and temporally, complicating the determination of the neutral-ion overlap and the extracted rate coefficient; (5) The energy of the carbon atoms and the energy spread of the effusive beam are both highly uncertain; and (6) The greater than 3000 K kinetic temperature of the carbon atoms is one to two orders of magnitude higher than typical molecular cloud temperatures.

3. Proposed Research, Instrument Description, and Feasibility Analysis

We propose to develop and construct a new and unique laboratory instrument to study reactions of molecular ions with neutral atomic C. Beginning with a C^- beam, we will use laser photodetachment to produce neutral ground term $C(^3P)$. Electrostaticly removing the remaining C^- will give us a pure C beam. Our apparatus will be unique for being able to produce a controlled pure C beam with insignificant internal energies which could otherwise alter the reaction chemistries to be studied.

Studies of reaction 1 will be carried out for the proof-of-principle. A beam of H_3^+ ions will be merged with the C beam to be co-linear and co-propagating. Both beams will be traveling at keV lab energies, allowing for ease of handling and easy beam profile measurements. Because the beams are co-propagating, this will allow us to study reactions from meV to keV center-of-mass energies (i.e., down to effective temperatures on the order of ~ 100 K and possibly lower). Reaction channels will be studied using a charge-to-mass analyzer to separate and detect the charged end products. Measuring all the relevant currents, beam shapes, energies, signal counts, and background rates will allow us to determine absolute cross sections for both reactions.

This research lies at the intersection of astronomy, biology, chemistry, and physics. Development of this novel technology will be followed by many years of research studying the 90+ ion-neutral reactions involving atomic C needed to interpret molecular spectra from

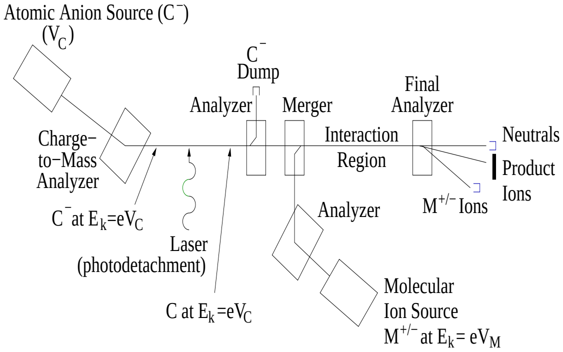

Figure 3: Schematic overview of our proposed novel research instrument. For clarity we have not shown in the drawing the various vacuum pumps, ion optic elements, beam profile monitors, and other details. The diagram is not to scale.

cosmic objects (Woodall et al. 2007). Additionally, the negative ion source used to generate C^- can also produce O^-. With a suitably chosen laser, ground term $O(^3P)$ beams can be produced via photodetachment and studies carried out for many of the 80+ ion-neutral reactions involving atomic O in current astrochemical databases (Wakelam et al. 2006a; Woodall et al. 2007), many of which lead to organo-oxygen compounds (Herbst & Leung 1989).

3.1 Producing the Neutral Beam

Figure 3 shows the proposed instrument which begins with a commercially available Peabody Scientific negative ion sputter source. Singly-charged carbon anions C^- are extracted from the source and accelerated to an energy $eV_C = 30$ keV. To remove any unwanted anions or electrons which have also been accelerated, the C^- beam is charge-to-mass selected using a dipole magnet. This will remove contaminants such as $^{12}CH^-$ and $^{13}C^-$ yielding a pure $^{12}C^-$ beam. Our experimental tests with a commercially available crossed electric and magnetic fields filter (a Wien filter) show that it cannot adequately resolve these beams.

The ion source is specified to produce 250 μA beams of C^- at 30 keV. The measured emittance of the ion source at 30 keV is 87 π mm mrad (Zarcone et al. 1993). Our goal is to transport to the C^- photodetachment region a beam with a radius of 2.5 mm and divergence of 3.5 mrad ($\Delta\theta = 0.2°$) giving an effective acceptance of 8.8 π mm mrad. Multiplying the source output current by the square of the ratio of the acceptance to the emittance (Humphries 1990) shows that we can expect to be able to transport a C^- beam of ≈ 2.6 μA to the photodetachment chamber.

C^- is one of the rare atomic anions which possess more than one stable bound level lying below the first detachment threshold: a ground $2s^22p^3$ $^4S_{3/2}$ level and the two excited $2s^22p^3$ $^2D_{5/2,3/2}$ levels. However, sputter sources such as we will use have been shown to produce insignificant populations amounts of the ^2D_J levels (Scheer et al. 1998; Takao et al. 2007). Thus we will produce an essentially pure beam of ground level C^-.

The C^- beam will be crossed with a commercially available 808 nm (1.53 eV) DILAS Inc. diode laser beam to photodetach and neutralize some of the C^- beam. The photodetachment cross section is well known experimentally and theoretically in the energy region of interest here (Seman & Branscomb 1962; Zhou et al. 2004).

Photodetachment of $^4S_{3/2}$ C^- using a 1.53 eV laser beam will produce ground term $C(^3P)$. Based on the work of Scheer et al. (1998), we expect that all three J levels of the ground term will be populated. The $J = 1$ and 2 levels lie above the $J = 0$ ground level by 2.0 meV ($k_BT_e \approx 16$ K) and 5.4 meV (42 K), respectively (recalling that in a gas $< E >= \frac{3}{2}k_BT_e$). These internal energies are a factor of over 230 times smaller than that achievable using the electron capture method (see §2) but are comparable to the molecular cloud temperatures. This will help us to mimic molecular cloud conditions. Such small internal energies are expected to have an insignificant effect on the exothermic reactions we plan to study.

We can estimate the expected neutral C beam produced via photodetachment. The diode laser can produce a beam 2.5 mm high and 15.0 mm wide at the focus. Approximating our C^- beam with a square profile 5 mm by 5 mm gives a photodetachment efficiency factor of

$$f = 2\sigma_{pd}\left(\frac{P_\gamma}{E_\gamma}\right)\left(\frac{1}{v_{\mathrm{C}^-} h_{\mathrm{C}^-} \sin\theta}\right) \approx 0.14 \ (14\%) \tag{5}$$

where the photodetachment cross section $\sigma_{pd} \approx 1.5 \times 10^{-17}$ cm^2, the laser power $P_\gamma \approx 2$ kW, the energy per photon $E_\gamma \approx 2.5 \times 10^{-19}$ J, the C^- beam velocity $v_{\mathrm{C}^-} \approx 7 \times 10^7$ cm s^{-1}, the C^- beam height $h_{\mathrm{C}^-} \approx 0.5$ cm, and the intersection angle $\theta \approx 2.73°$. The shallow intersection angle increases f by increasing the overlap length. The factor of 2 arises because we will pass the laser beam twice through the C^- beam. Thus we expect to be able to produce a 30 keV C beam with a particle current of ≈ 364 nA and a height of 2.5 mm.

3.2 Molecular Ion Source

The proof-of-principle measurement will use a commercially available Peabody Scientific duoplasmatron source to generate an H_3^+ beam. We will extract the beam at an energy of $eV_M \approx 7.5$ keV. This will nearly match the velocity of the C beam and achieve the low relative velocities required to study collisions at molecular cloud temperatures.

At a beam energy of ≈ 7.5 keV, the duoplasmatron outputs a 20 μA H_3^+ beam with an emittance of 74 π mm mrad. Our goal is to transport into the interaction region an H_3^+ beam with a radius of 2.5 mm and divergence of 3.5 mrad ($\Delta\theta = 0.2°$) giving an effective acceptance of 8.8 π mm mrad. Multiplying the source output current by the square of the ratio of the acceptance to the emittance tells us that we expect to be able to transport an H_3^+ beam of ≈ 283 nA into the interaction region.

3.3 Interaction and Analyzer Regions

We will electrostaticly merge the H_3^+ beam with the C beam so they co-propagate at low relative energies for a distance $L \approx 100$ cm. This portion of the apparatus will be surrounded by magnetic coils to cancel the deflection of the H_3^+ beam by the Earth's magnetic field. In the interaction region, the two beams will undergo chemical reactions. The primary beams and product beam (here CH^+) will then be separated from the neutrals and from one another using a dipole magnet. The ≈ 50 cm flight distances after this magnet will be long enough to provide separation on the order of centimeters between all beams, parent and product. This will also separate from the CH^+ beam any C^+ created by stripping of the parent C beam on rest gas. In this way we will be able to cleanly resolve and detect each beam. The neutral and primary beams are directed into separate Faraday cups located in separate beam dump chambers. The neutral beam particle current will be measured indirectly through the secondary electron emission generated by the C beam striking the Faraday cup. The arrangement of dump chambers separated from the analyzer region will decrease the likelihood of photons or particles produced by the beams striking the Faraday cups from making their way into the product ion detectors, thereby reducing the background.

Product ions will undergo two additional 90° electrostatic deflections to further reduce particle and photon backgrounds. The first deflection will be perpendicular to the dispersion plane of the magnet and the second perpendicular to the dispersion planes of both the magnet and the first electrostatic deflection. The surfaces of the electrostatic deflectors will be coated with carbon to blacken them and reduce the reflectance for any beam-generated background photons. Our experience with detecting charged particles from merged beams systems has shown that this arrangement can reduce beam-generated background rates to essentially zero. Product ions will be directed onto detectors running in particle counting mode.

We will use standard beam chopping techniques to collect data and extract the signal from the background (Phaneuf et al. 1999). The C beam will be modulated by chopping the laser. The H_3^+ beam will be chopped using an electrode just after the molecular ion source. Beam profiles and particle densities will be measured at 4 positions along the interaction region. Commercially available devices will be used. The entire beam-beam overlap will be calculated at these 4 positions along the overlap region and interpolated between these positions. Measuring all the relevant currents, beam shapes, energies, background rates, and signal count rates will allow us to determine absolute reaction cross sections. Based on our experience with merged-beams experiments (Savin et al. 1997; Seredyuk et al. 2007a; Savin et al. 2008), we expect to be able to measure absolute cross sections with a total systematic plus statistical accuracy of $\sim 27\%$ at a 90% confidence level (see §3.5).

3.4 Signal Rate and Data Acquisition Time

The signal rate R_{sig} can be estimated assuming square beams. An atomic C beam of height $h_1 \approx 2.5$ mm and width $w_1 \approx 5.0$ mm and an H_3^+ beam of $h_2 = w_2 \approx 5.0$ mm give

$$R_{sig} = \sigma_{sig} v_r \int n_1 n_2 dV \approx \sigma_{sig} \left(\frac{v_r}{v_1 v_2} \right) \left(\frac{I_1 I_2}{e^2} \right) \left(\frac{L}{h_2 w_2} \right) \tag{6}$$

where σ_{sig} is the cross section for the reaction of interest; v_r is the center-of-mass relative velocity between the beams; n_1 and n_2 are the densities of the C and H_3^+ beams, respectively; v_1 and v_2 are their respective laboratory velocities; I_1 is the C beam particle current expressed in units of electrical current; I_2 is the H_3^+ current; $e = 1.6 \times 10^{-19}$ C is the electrical charge; and L is the overlap length.

The rate coefficient for reaction 1 at 300 K is $\sigma_{sig} v_r \sim 1 \times 10^{-9}$ cm^3 s^{-1}. The laboratory velocities of the beams are nearly matched at $v_1 \approx v_2 \approx 7 \times 10^7$ cm s^{-1}. From above we have, $I_1 = I_{\mathrm{C}} \approx 364$ nA, $I_2 = I_{H_3^+} \approx 283$ nA, and $L \approx 100$ cm. Putting it all together yields a predicted signal rate of $R_{sig} \approx 330$ s^{-1} with an estimated factor of 10 uncertainty due to the range in the theoretical and experimental rate coefficient for reaction 1 and the approximation of using square beams with uniform particle densities.

We will use standard chopping procedures for the two beams in order to extract the signal from the various backgrounds in the experiment (Phaneuf et al. 1999) with a resulting duty cycle of ≈ 1/5th (20%). The time t required to collect data at a 1σ counting statistical accuracy of $A = 0.25$ (25%) is

$$A = \frac{\sqrt{(S+B)t}}{\frac{1}{5} S t} \Rightarrow t = \frac{400(S+B)}{S^2} \tag{7}$$

where S is the signal rate and B the background rate.

Data acquisition time will be limited by the actual CH^+ signal rate, which we estimate to range between $33 - 3300$ s^{-1}, and the unknown background rate. Using a pure parent beam of $^{12}C^-$ will insure that there is no ^{12}CH or ^{13}C produced in the neutral beam which could be ionized by the rest gas in the vacuum system and create an ion with the same charge-to-mass ratio as the signal $^{12}CH^+$. Reactions of the C or H_3^+ beams with residual gas in the vacuum system will be unable to produce a beam of $^{12}CH^+$ at the appropriate energy for detection. Thus, we expect the background will less than 1 s^{-1} and the estimated data acquisition time to range between $\approx 0.12 - 12$ s. The most likely sources of background are photons or charged particles produced by the parent ions striking metal surfaces when the beams are collected and the currents measured in their respective dumps. We will design the end stage of the experiment to minimize any such particle background. For the sake of argument, if $B = 100$ s^{-1}, then the required data acquisition time ranges between $\approx 0.12 - 49$ s which is still sufficiently short as to allow us to rapidly troubleshoot the apparatus.

3.5 Predicted Uncertainties

For our absolute measurement of σ_{sig} using Eq. 6, the major uncertainties are predicted to be as follows: H_3^+ current (8%), C current (10%), interaction length (15%), overlap determination (10%), product ions detector (8%), background determination from beam chopping (8%), and counting statistics (10%). These are all based on our previous work (Seredyuk et al. 2007a; Savin et al. 2008) and are quoted at a 90% confidence limit. Treating all as random sign uncertainties and adding in quadrature yields an expected accuracy of 27% (16% at a 1σ level).

3.6 Advantages of Our Approach Relative to Previous Work

Our approach will not suffer from the limitations of past methods. Our C beam will consist of ground term atoms with insignificant internal energies. Each beam will have no contaminants which could react with the C or H_3^+ and complicate the data analysis. Neither ion source will have a direct line of sight to the interaction region, so VUV radiation from the sources altering the chemistry studied is not an issue. Studies will be carried out in the single collision regime, preventing parasitic reactions. The ion sources emit beams at nearly constant currents as opposed to in bursts. The energy of each beam will be high enough to use standard beam profile measurements to determine their spatial densities (Seely et al. 2008). The acceleration energies will be well known allowing for a reliable center-of-mass collision energy E_{cm} determination. Initial measurements will reach temperatures a factor of > 5 below those of the high temperature carbon rod vaporization method.

4. Resources Required

The total budget for the three years of the proposed research is \$1,993,831. This sum includes \$801,096 for salaries and fringe benefits; \$918,852 for equipment; \$102,074 for materials, supplies, page charges, travel, tuition, etc; and \$171,809 for indirect costs.

Personnel for the project include the PI, Dr. Daniel Wolf Savin, an Associate Research Scientist, a Postdoctoral Research Scientist, a Graduate Student, and an Undergraduate Student, all of whom will participate in designing and building the proposed new technology.

Equipment purchases include 2 dipole magnets (\$182,600); 8 turbomolecular pumps (\$149,424); 2 ion sources (\$115,520); a photodetachment laser (\$96,230); data acquisition electronics, oscilloscopes, and computer (\$74,318); and 7 beam profile monitors (\$31,500). The remaining $\sim \$270,000$ includes power supplies, vacuum chambers and hardware, feedthroughs, manipulators, support structures, and other general laboratory needs.

This novel instrument will be built in the 2000 sq. ft. laboratory space provided for Dr. Savin's use by the Columbia Astrophysics Laboratory. The space is located in the Cyclotron

Building at Nevis Laboratories which is part of Columbia University.

5. The Reason Why a Targeted Investment is Needed

Our proposed astrobiology technology development is urgently needed for interpreting the molecular cloud spectra which will be collected in the coming decade. However, a source of funding for this project remains to be found. The level of support required exceeds by a factor of ~ 6 the average grant awarded by programs which have traditionally supported laboratory astrophysics such as the NASA Astronomy and Physics Research and Analysis (APRA) program and the NSF Astronomy and Astrophysics Grants (AAG) program. Our proposed astrobiology research also falls outside the mandate or funding history for those NASA and NSF programs which could potentially provide support at the level required for the proposed instrument development. The NASA Astrobiology Science and Technology Instrument Development (ASTID) program is for satellites, payloads, and flight hardware. The NSF Division of Astronomical Sciences Advanced Technologies and Instrumentation (ATI) program has historically supported only development of equipment and detectors which can be attached to telescopes. Neither program has funded laboratory astrophysics; and, not surprisingly, our proposal has been declined by each program. Progress in this critically needed area of astrobiology will come about only with a targeted investment in the development of our proposed ground breaking technology.

6. Milestones

Our previous experience developing and operating merged beams experiments (e.g., Savin et al. 2008) has allowed us to develop the expertise necessary to build the proposed apparatus and to accurately estimate the time required taking into account issues such as the long lead time for many purchases, time needed to design the new portions of the apparatus, machining time required, construction and assembly time, testing, etc.

Year 1: Develop the first leg of the neutral beam line and the molecular ion beam line.

Year 2: Develop the photodetachment section of the neutral beam line and associated parent ion beam dump. Develop the merging portion and interaction region of the apparatus.

Year 3: Develop the final products analyzer, detectors, and beam dumps. Debug the apparatus and begin to collect data.

It is important to note that we are not proposing to add just one new measured rate coefficient to the large set of processes in the reaction network. Rather, with our new experimental approach an entire new class reactions will become accessible for laboratory measurements, thereby improving our understanding of chemistry in cold environments.

Additionally, astrochemistry requires reaction data not just at the low temperatures relevant for molecular clouds but specifically for reactions involving cold molecules with internal energies similar to what is observed. That is our ultimate goal and we have taken a two step approach to reach it. The first step, described above, will achieve cold collisions with cold C atoms but will be carried out using a hot molecular ion source. This will already represent a major advance in the ability to carry out laboratory simulations of molecular cloud chemistry. The second step (after completion of this proposal) will be to install a cold molecular ion source similar to the pulsed cold molecular ion source of McCall et al. (2004) which has recently been modified to operate in continuous mode (McCall 2008).

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