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Isomer-specific kinetics of the C+ + H2O reaction at the temperature of interstellar clouds

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The reaction C+ + H2O → HCO+/HOC+ + H is one of the most important astrophysical sources of HOC+ ions, considered a marker for interstellar molecular clouds exposed to intense ultraviolet or x-ray radiation. Despite much study, there is no consensus on rate constants for formation of the formyl ion isomers in this reaction. This is largely due to difficulties in laboratory study of ion-molecule reactions under relevant conditions. Here, we use a novel experimental platform combining a cryogenic buffer-gas beam with an integrated, laser-cooled ion trap and high-resolution time-of-flight mass spectrometer to probe this reaction at the temperature of cold interstellar clouds. We report a reaction rate constant of k = 7.7(6) × 10^{-9} cm^3 s^{-1} and a branching ratio of formation η = HOC+ / HCO+ = 2.1(4). Theoretical calculations suggest that this branching ratio is due to the predominant formation of HOC+ followed by isomerization of products with internal energy over the isomerization barrier.

Advanced experimental techniques developed in atomic physics for preparation of ultracold matter and quantum information science have recently been adapted to chemical studies. While these techniques allow preparation and coherent control of a reagent in single internal and external quantum states, they have, so far, been limited to a narrow range of species, e.g., the alkali atoms. As a result, despite groundbreaking work that has assembled single molecules (7), observed a conformer-dependent reaction (8), and produced novel molecules (9), no study to date has adapted these techniques to a reaction where all reagents are chemically relevant. Here, we develop a novel experimental platform based on these atomic physics techniques that allows studies of reactions of virtually any atomic ion with a wide range of neutral molecules. Specifically, we combine a laser-cooled ion trap with integrated mass spectrometer (MS) and cryogenic buffer-gas beam (CBGB) (Fig. 1A). These tools have been independently used in a number of pioneering studies (8–12), but they have typically been restricted to laser-cooled atomic reagents and produce reagents at temperatures substantially colder than the interstellar medium (ISM). In this work, we adapt them to produce C+ and H2O at more characteristic temperatures (∼20 K) to properly simulate cold interstellar clouds in the laboratory.

Using this platform, we study the reaction C+ + H2O → HOC+/ HCO+ + H with product isomer specificity under conditions relevant to those in cold molecular clouds. This reaction is believed to be the chief source of the metastable ion HOC+, which has been observed in a variety of sources including of nearby PDRs (13), toward our own galactic center (14, 15), in the early starburst galaxy M82 (16, 17), a later starburst galaxy NGC 253 (18), in the ultraluminous infrared galaxy Mrk273 (19), and in the AGNs of NGC 1068 and other active galaxies. The lower-energy isomer HCO+, on the other hand, is largely formed via protonation of CO by the ubiquitous ion H+3, and it is generally far more abundant. The relative abundance of HCO+ to HOC+ is seen to vary by many orders of magnitude, from well over 10^4 in the weakly irradiated PDR S140 (13) to 10 in the inner CND of Mrk273 (19). One question is, To what extent can HOC+ serve as a specific marker for XDRs (3)? A recent survey toward two quiescent cloud complexes of the galactic center, one of which is likely exposed to strong x-ray radiation, suggested that the CS/HOC+ ratio was a reliable marker for PDR/XDR components in...
galactic tracer useful to distinguish PDR and XDR regions (20). For models to be used reliably to reveal conditions in distant molecular clouds in these very diverse environments, the yield of the associated reactions must be accurately known. These relative abundances obviously depend on the product branching ratios of the underlying chemical reactions that produce these molecules (13, 21). For the title reaction, the product channels are

\[
\begin{align*}
C^+ + H_2O & \rightarrow HOC^+ + H \\
C^+ + H_2O & \rightarrow HCO^+ + H
\end{align*}
\]

(1, 2)

Hence, the rate and branching ratio, \( \eta = HOC^+/HCO^+ \), of this reaction has attracted significant interest over the past 30 years; however, there is still no consensus on the latter value and it has never been measured at low temperature (22–26). Freeman and McEwan (22) investigated this reaction with a selected-ion flow tube (SIFT) at room temperature and reported \( \eta = 5(2) \) by using the different proton transfer rates of the isomers with \( N_2O \) to distinguish \( HCO^+ \) from \( HOC^+ \). Martinez and co-workers (27) more recently studied the reaction using the flowing-afterglow-SIFT technique to eliminate the contribution of electronically excited \( C^+ \) ions but did not measure branching and quite reasonably assigned all the products to \( HOC^+ \). Sonnenfroh et al. (25) carried out a crossed-beam experiment to study this reaction at collision energies of 0.62 and 2.14 \( eV \), in which they concluded that \( \eta \leq 2.3 \) and pointed out that the high internal temperature of the products due to the exothermicity of the reaction (\( \Delta H = -4.34 \text{ eV} \)) may affect the identification of the isomers in subsequent titration reactions. In theoretical calculations, Defrees et al. (28) used phase-space arguments to calculate \( \eta = 2 \). However, using quasi-classical trajectory (QCT) studies, Ishikawa et al. (29) found that \( HOC^+ \) dominated the initial products of the reaction giving \( \eta \approx 100 \). The authors discussed the possibility of subsequent isomerization due to internal energy of the products to explain the existence of \( HCO^+ \) in experimental observations; however, no calculations for the isomerization rate were performed. Despite these disagreements, the room temperature measurement of \( \eta = 22 \) has been widely used to understand ISM chemistry and classify PDRs for decades (13).

Here, we build on pioneering work of Gerlich and others (30–32) and report the first study of the \( C^+ + H_2O \) reaction under conditions present in cold molecular clouds of the ISM. We find the reaction proceeds with a rate constant of \( k = (7.7(6) \times 10^{-9} \text{ cm}^3 \text{ s}^{-1} \) at \( \approx 20 \text{ K} \), slightly lower than the value reported at 27 K (26). Titrating the reaction products with \( ^{15}N_2 \), which reacts with \( HOC^+ \) but not \( HCO^+ \), we measure the ratio of \( HOC^+ \) to \( HCO^+ \) exposed to the titrant to be 1.4(2). Accounting for isomerization during the titration process, we report \( \eta = 2.1(4) \). QCT calculations on an accurate potential energy surface (PES) found that the \( C^+ + H_2O \) reaction produces 97.6\% \( HOC^+ \), of which 87.8\% of these products are produced with an internal energy above the isomerization barrier. We calculate that the
density of HOC⁺ vibrational states is twice that of HCO⁺ near the isomerization barrier. Therefore, we expect that roughly two-thirds of the above-barrier products decay to HCO⁺, which modifies the predicted branching ratio to \( \eta = 2.3 \), in agreement with the experiment.

**MATERIALS AND METHODS**

A schematic of the apparatus used in this study is shown in Fig. 1A. Briefly, an integrated laser-cooled ion trap and time-of-flight (TOF)-MS (33), which has been described in detail elsewhere (34, 35), is combined with a CBGB (18). Laser ablation of beryllium and graphite is used to simultaneously produce Be⁺ and C⁺ ions, which are trapped in a linear radio frequency Paul trap. Laser cooling (36) is used to cool the translational motion of the Be⁺ ions, which sympathetically (37, 38) cools the cotrapped C⁺ ions to <1 K. This process takes several seconds; during that time, any metastable \((^3\text{P})\) C⁺, which may have plagued other measurements as explained in (27), spontaneously relaxes (39). Water vapor is entrained in the neon CBGB (40), which is cooled by a closed-cycle refrigerator to 20.0(5) K, and directed toward the center of the ion trap with a forward velocity of 150(2) m/s (see the Supplementary Materials) to facilitate C⁺ + H₂O reactions. The reactions occur inside the ion trap, which is held in a high vacuum chamber (<5 × 10⁻¹⁰ mbar) (34, 35), and the trapped ionic reactants and products are analyzed by an integrated TOF-MS (9, 41, 42).

Two isomers of the formyl ion, HCO⁺ and HOC⁺, are produced in this reaction; however, TOF-MS is unable to distinguish these ions as they have the same mass and charge. To distinctly titrate the HCO⁺ in this reaction; however, TOF-MS is unable to distinguish these ions (Fig. 1D), reactions 3 and 4 are validated. Unfortunately, the mass of diazenylium \((^{14}\text{N}_2\text{H}^+)\), \(m_D = 29.01\) atomic mass units (amu), is nearly equal to that of the formyl ion, \(m_F = 29.00\) amu, and these products cannot be resolved by our MS. Therefore, we use \(^{15}\text{N}_2\) as a titrant gas to produce diazenylium with a mass of 31.01 amu, which is easily resolved by our MS. Reaction 4 has been validated experimentally, as shown in Fig. 1D.

The experimental sequence is described in the Supplementary Materials. Briefly, trapped C⁺ ions are sympathetically cooled by the cotrapped Be⁺ ions. Next, the H₂O beam is introduced into the trap for 20 s and reactions occur. After an approximately 1-s delay to allow the internally excited product ions to isomerize and/or relax via radiative decay (43), the \(^{15}\text{N}_2\) titrant gas is introduced for approximately 10 s. Afterward, all ions are ejected into the TOF-MS, and Fig. 1B shows a typical TOF signal. From these data, we find the reaction rate constant \(k_1 + k_2 = 7.7(6) \times 10^{-9} \text{cm}^3/\text{s}^{-1}\) (see section S3 for the details).

Several other species, not studied here, are also apparent in the TOF-MS signal. These are understood as follows. Be⁺ ions are known to react with H₂O to make BeOH⁺ and a small amount of H₂O³⁺ (34, 35). Most of the H₂O³⁺ comes from the reactions

\[
\text{HCO}^+ + \text{H}_2\text{O} \rightarrow \text{H}_3\text{O}^+ + \text{CO} \quad (5)
\]

\[
\text{HOC}^+ + \text{H}_2\text{O} \rightarrow \text{H}_3\text{O}^+ + \text{CO} \quad (6)
\]

\[
\text{HOC}^+ + \text{CO} \rightarrow \text{HCO}^+ + \text{CO} \quad (7)
\]

The rate coefficient of reaction 5 has been measured as \((2.5 \pm 0.3) \times 10^{-9}\text{cm}^3/\text{s}\) at 300 K (44), but not at lower temperature. Although the appearance of H₂O³⁺ presents no problem for our study, a relative rate difference between these two reactions (5 and 6) at low temperature would systematically shift the trapped HOC⁺/HCO⁺ ratio and cause an error in the determination of branching ratio \(\eta\). To constrain this potential error, we introduced CO to produce samples with varying compositions of HCO⁺ and HOC⁺ (details can be found in the Supplementary Materials) from the reaction

\[
\text{HOC}^+ + \text{15}\text{N}_2 \rightarrow \text{HCO}^+ + \text{15}\text{N}_2 \quad (8)
\]

We find \(k_5 \approx k_6 = (1.7 \pm 0.2) \times 10^{-9}\text{cm}^3/\text{s}\), and therefore, the HOC⁺/HCO⁺ ratio is not measurably affected.

Therefore, since isomerization of the isoformyl ion by H₂O does not occur (45) (see the Supplementary Materials), the branching ratio of HOC⁺ and HCO⁺ can be inferred from the ratio of the integrated mass/charge ratio \((m/z = 31.01\text{amu}/e(\text{^{15}\text{N}_2\text{H}^+}))\) and \(m/z = 29.00\text{amu}/e\) (HCO⁺) peaks in the TOF signal, which is found to be 1.4(2). Repeating this process over various densities (Fig. 1C) of \(^{15}\text{N}_2\) allows us to confirm this measurement as well as determine the proton transfer rate constant of reaction 3 to be \(k_3 = 6.6(1) \times 10^{-10}\text{cm}^3/\text{s}\) (see the Supplementary Materials).

In addition, to verify that \(^{15}\text{N}_2\) is only able to react with HOC⁺ and not HCO⁺. We repeat the above process in the presence of a large amount of neutral CO gas for converting all of the HOC⁺ to HCO⁺ via the isomerization reaction 7 and then introduce excess \(^{15}\text{N}_2\). Since there is no evidence of \(m/z = 31.01\text{amu}/e(\text{^{15}\text{N}_2\text{H}^+})\) in the TOF trace (Fig. 1D), reactions 3 and 4 are validated.

**RESULTS**

Before the branching ratio \(\eta\) can be extracted from the measured product ratios, it is necessary to account for isomerization by the titrant gas, i.e.

\[
\text{HOC}^+ + \text{15}\text{N}_2 \rightarrow \text{HCO}^+ + \text{15}\text{N}_2 \quad (8)
\]

As HCO⁺ is unreactive to \(^{15}\text{N}_2\) at these temperatures, this reaction artificially lowers the measured branching ratio. To understand this effect, QCT calculations (46) on an long-range corrected ab initio PES for the HOC⁺ + \(^{15}\text{N}_2\) system were performed (47). These calculations yield a 14% isomerization (see the Supplementary Materials) fraction. The isomerization fraction can be constrained with the assumption that the total rate constant for HOC⁺ + \(^{15}\text{N}_2\) is given by the Langevin capture rate constant, \(k_1 = 8.0 \times 10^{-10}\text{cm}^3/\text{s}\). Thus, the measured value of \(k_5\) suggests a possible isomerization fraction of up to 18%. Using the isomerization rate found in the QCT calculations, the measured reaction branching ratio becomes \(\eta = 2.1(4)\).

**DISCUSSION**

To better understand this reaction, a six-dimensional global PES for reactions 1 and 2 was constructed from the explicitly correlated unrestricted coupled cluster singles, doubles, and perturbative triples [UCCSD(T)-F12a] calculations (details of ab initio calculations and fitting are given in the Supplementary Materials). The energetics for
reactions 1 and 2 are shown in Fig. 2. As C$^+$ approaches water, it can be transiently trapped in the IM1 (Intermediate 1) well, in which C is bonded to O. Given the system energy, however, the intermediate is relatively short lived and not significantly affected by the two transition states. Because of the large frequency mismatch among its vibrational modes, the vibrational energy is hardly randomized in the intermediate. In most cases, the large energy in the C transition states. Because of the large frequency mismatch among its is relatively short lived and not significantly affected by the two bond results in HOC$^+$, lowering the predicted branching ratio to $\eta = 2.3$.

Interstellar molecular clouds ultimately yield the seedbed from which new stars and planets are born, as well as the raw materials from which life likely developed. Thus, understanding the chemical evolution of the ISM is essential to understanding these important processes. Chemical reaction rates and branching ratios underlying models of this evolution are often (necessarily) taken from experiments and theory that are not appropriate for the conditions present in cold molecular clouds. The apparatus used here is quite versatile and could be applied in its present form to study most atomic ion–neutral molecule reactions under conditions relevant to cold molecular clouds of the ISM chemistry.

**SUPPLEMENTARY MATERIALS**

Supplementary material for this article is available at http://advances.sciencemag.org/cgi/content/full/7/2/eabe4080/DC1

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