

Formation of Carbonisocyanatidic Amide in Interstellar Ice Analogs as a Candidate Precursor to Prebiotic Pyrimidines

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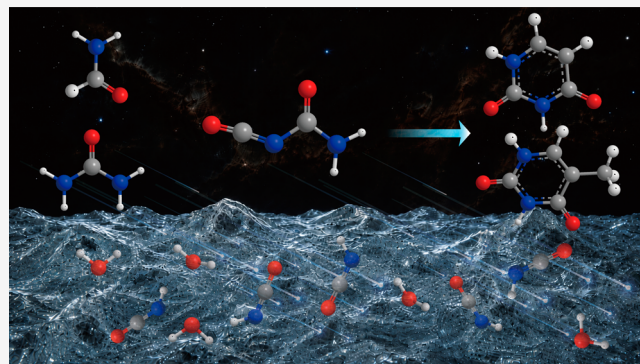


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ABSTRACT: Understanding how pyrimidine nucleobases form in space is central to prebiotic chemistry, yet the pathways assembling these heterocycles remain unresolved. Carbonisocyanatidic amide ($\text{H}_2\text{NC(O)NCO}$), an acyclic intermediate with heteroatom connectivity relevant to uracil and thymine, has not been detected in interstellar ice analogs. Here, we show that carbonisocyanatidic amide is formed in low-temperature isocyanic acid (HNCO) ices exposed to energetic electrons and is identified during the desorption phase by synchrotron vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry combined with high-level quantum chemical calculations. A plausible, product-constrained network involves hydrogen abstraction and addition steps that generate radical intermediates, followed by radical–radical recombination and carbon–nitrogen bond formation. These results establish an experimental link between simple interstellar volatiles and nitrogen-rich molecular architectures relevant to pyrimidine nucleobases, supporting an astrochemical route to prebiotic intermediates in icy grains and their possible delivery to early Earth.



Elucidating the origin of genetic biomolecules remains a central challenge in prebiotic chemistry and astrobiology.^{1,2} Deoxyribonucleic acid (DNA) and ribonucleic acid (RNA) encode and transmit biological information, and their pyrimidine nucleobases (uracil, thymine, and cytosine) are essential building blocks,^{3,4} yet the abiotic routes leading to these six-membered nitrogen-containing heterocycles remain poorly understood.⁵ Astronomical observations and meteoritic analyses have revealed a growing inventory of nitrogen-bearing, biologically relevant organic molecules in extraterrestrial environments, including carbonaceous meteorites (such as Murchison and Murray), comets (e.g., 67P/Churyumov–Gerasimenko), and the interstellar medium (ISM).^{6–9} Notably, nucleobases including uracil and thymine have been detected both in carbonaceous chondrites and in pristine samples recently returned from carbonaceous asteroids Bennu and Ryugu.^{6,8,10,11} These discoveries indicate that biologically relevant organic molecules can form in extraterrestrial environments and survive delivery to planetary surfaces. Carbonisocyanatidic amide ($\text{H}_2\text{NC(O)NCO}$) contains a contiguous NC(O)NCO atom sequence corresponding to the $\text{N1–C2(=O)–N3–C4(=O)}$ segment of the pyrimidine-2,4-dione ring in uracil and thymine. Completion of this framework would require incorporation of a suitable two-carbon unit and formation of the C4–C5 and C6–N1 bonds, while formation of thymine would additionally require introduction of the C5 methyl group. Synthetic studies have

shown that one alkyne and two isocyanates can be cocyclized to pyrimidine-2,4-diones^{12,13} and into uracil- or thymine-containing rings by trapping an isocyanate intermediate with lithium salts of acrylic amides followed by cyclization.¹⁴ Related reactions with enamionitriles and alkyne-tethered malononitriles further demonstrate the broader role of isocyanates in pyrimidinone construction.^{15,16} These precedents suggest that carbonisocyanatidic amide may represent a structurally preorganized intermediate for subsequent pyrimidine-forming chemistry and provide a chemical basis for examining the molecular growth of HNCO -derived N–C–O skeletons during energetic processing of more complex ices and later chemical evolution.

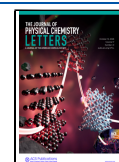
Laboratory simulation experiments demonstrate that galactic cosmic ray (GCR) processing of interstellar ice analogs drives rich, nonequilibrium reaction networks. Energetic irradiation by GCRs, ultraviolet photons, and secondary electrons generates reactive radicals, enabling bond-forming reactions inaccessible under thermal conditions.^{17–19} Such processes

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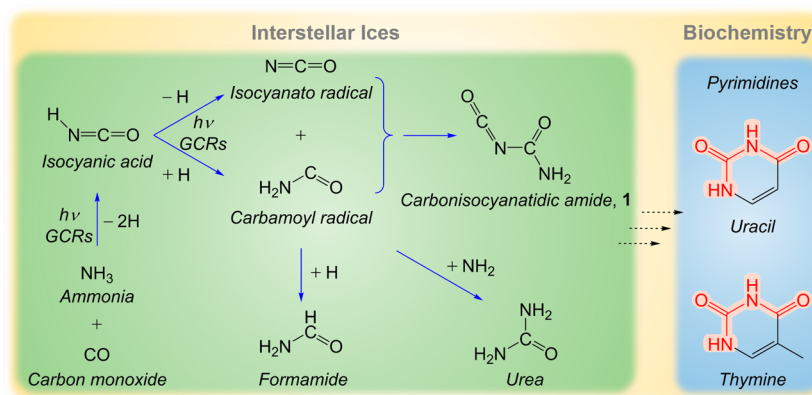


Figure 1. Proposed formation of carbonisocyanatidic amide ($\text{H}_2\text{NC}(\text{O})\text{NCO}$, **1**) in energetically processed HNCO-rich interstellar ice analogs and its potential connection to pyrimidine chemistry. Energetic processing generates the isocyanato (NCO) and carbamoyl (H_2NCO) radicals through H atom loss from and addition to HNCO, respectively. Their recombination forms the central N–C bond of **1**, while related radical pathways to formamide and urea are also shown. The dotted arrows indicate the potential of **1** to enter subsequent pyrimidine-forming chemistry with suitable carbon-bearing reaction partners, rather than specific conversions demonstrated in the present study.

have been shown to yield a wide range of biologically relevant compounds, including amino acids, sugars, nucleobases, and dipeptides.^{17,18,20} Notably, the condensation of atomic carbon with carbon monoxide (CO) and ammonia (NH_3) yields aminoketene intermediates, which undergo spontaneous polymerization to form peptide-like oligomers.²¹ Small nitrogen-bearing carbonyl compounds (isocyanic acid (HNCO), formamide (H_2NCHO), urea ($\text{NH}_2\text{C}(\text{O})\text{NH}_2$), ammonium cyanate ($\text{NH}_4^+\text{OCN}^-$)) occupy a central role in interstellar ice chemistry.²² HNCO has been widely detected toward sources Sgr B2(N) and TMC-1,²³ as well as in comets,²⁴ and serves as a versatile building block capable of hydrogen addition, nucleophilic attack, and tautomerization.^{25–27} Experimental astrochemical studies have shown that irradiated HNCO– H_2O and HNCO– NH_3 ices yield formamide, aminomethanol ($\text{NH}_2\text{CH}_2\text{OH}$), urea, carbamic acid ($\text{NH}_2\text{C}(\text{O})\text{OH}$), and diverse imino–oxo species.^{25,28,29} Haupa et al. further demonstrated that the near-equilibrium between H_2NCHO and HNCO is achieved through a dual-cycle mechanism of hydrogen abstraction and addition.²⁶ Despite this progress, the growth of larger N–C–O species from HNCO ice remains poorly characterized. Identifying such products is necessary to define the molecular inventory generated by energetic processing and to assess their possible roles in subsequent chemical evolution.

Here, we report the experimental detection of carbonisocyanatidic amide ($\text{H}_2\text{NC}(\text{O})\text{NCO}$) formed in HNCO ices upon electron irradiation, corresponding to an energy dose equivalent to approximately 1.5×10^7 years of processing in dense molecular clouds. This identification was achieved using synchrotron vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry (SVUV-PI-ReToF-MS) during temperature-programmed desorption (TPD), complemented by Fourier transform infrared spectroscopy (FTIR) of the solid-phase ice.^{30–34} Complementary quantum chemical calculations also predict an isomer-selective dissociative photoionization channel yielding H_2NCO^+ , consistent with the observed fragment associated with carbonisocyanatidic amide. Our results reveal that the energetic processing of HNCO ices under nonequilibrium conditions triggers a radical-mediated reaction mechanism, in which recombination of isocyanato (NCO) and carbamoyl (H_2NCO) radicals establishes the carbon–nitrogen scaffold of carbonisocyanati-

dic amide. This intermediate may be tested in reactions with unsaturated partners, such as acetylene (C_2H_2) and methylacetylene (C_3H_4), in multistep carbon-incorporation and ring-closure chemistry (Figure 1).^{35–37} The broader astrobiological context is illustrated by the recent analysis of pristine samples returned from carbonaceous asteroids Bennu and Ryugu, which reported the presence of canonical nucleobases, including uracil and thymine alongside a complex suite of nitrogen heterocycles.^{6,8,10,11} The identification of carbonisocyanatidic amide provides a molecular target for studying how simple interstellar N–C–O species grow into more complex pyrimidine-relevant structures. As an acyclic intermediate capable of further cyclization, condensation, and methylation, carbonisocyanatidic amide may provide a chemically accessible entry point to pyrimidine-forming chemistry under subsequent ice- or gas-phase processing. Once formed, it could be delivered to early Earth via comets and meteorites, offering a possible complement to RNA-world scenarios.^{10,38} Moreover, its distinct molecular structure makes it a promising target for remote detection of gas-phase molecules released from such ices, including in future observations with ground-based facilities such as the Atacama Large Millimeter/submillimeter Array (ALMA), and as a key tracer for forthcoming sample-return missions.

The chemical evolution of isocyanic acid ice during electron irradiation was monitored in situ by FTIR (Figure S1 and Table S1). The spectrum of pristine ice before irradiation (at 5 K) exhibited absorption peaks at $3496\text{--}2971\text{ cm}^{-1}$ (ν_1), 2237 cm^{-1} (ν_2), 1323 cm^{-1} (ν_3), and 886 cm^{-1} (ν_4), in agreement with the reported infrared spectrum of solid HNCO.³⁹ Upon electron irradiation, the after-minus-before difference spectrum displays negative features associated with depletion and irradiation-induced reshaping of the parent HNCO absorptions, together with positive features arising from newly formed products. The features in the $3470\text{--}3030\text{ cm}^{-1}$ region arise from decrease of the HNCO ν_1 band and formation of new N–H-bearing product.³⁹ The positive feature at 2341 cm^{-1} corresponds to the CO_2 ν_3 mode.⁴⁰ The 2310 cm^{-1} band corresponds to the asymmetric stretching mode of $-\text{N}=\text{C}=\text{O}$ groups.⁴¹ The absorption at 2160 cm^{-1} can be attributed to OCN^- .⁴² The band at 2139 cm^{-1} is assigned to the fundamental stretching vibration of CO , $\nu_{(\text{CO})}$.⁴³ The weak features at 2310 and 1457 cm^{-1} are tentatively assigned to the

asymmetric and symmetric stretching vibrations of the —N= C=O group, respectively, indicating the formation of one or more isocyanate-bearing irradiation products.⁴¹ The absorption at 1682 cm^{-1} is tentatively attributed to $\nu_{(\text{C=O})}$ of a carbonyl-bearing product.⁴¹ A weak feature at 1844 cm^{-1} is tentatively assigned to the CO stretching vibration of the formyl radical (HCO), which has previously been identified near $1842\text{--}1860\text{ cm}^{-1}$ in irradiated molecular ices.⁴⁴ The residual feature near 1333 cm^{-1} overlaps the parent HNCO ν_3 absorption and may originate from depletion or a small irradiation-induced frequency shift. The simultaneous observation of bands in the isocyanate and carbonyl stretching regions is compatible with the functional groups present in carbonisocyanatidic amide. Nevertheless, these frequency assignments are not unique to this structure, and contributions from other irradiation products cannot be excluded. Therefore, unambiguous confirmation of carbonisocyanatidic amide requires an alternative analytical technique capable of selectively identifying discrete isomers.

To identify carbonisocyanatidic amide, we combined isomer-selective SVUV-PI-ReToF-MS^{30–34} with the calculated adiabatic ionization energies (AIEs) for the six plausible $\text{C}_2\text{H}_2\text{N}_2\text{O}_2$ isomers (Figure 2 and Table S2). The TPD profiles of irradiated HNCO ices were analyzed in terms of the temperature and mass-to-charge ratio (m/z) using photon energies of 12.20, 11.00, 10.50, and 10.20 eV (Figure 3 and

Tables S3 and S4). Blank experiments performed under identical conditions but without radiation exposure yielded no detectable signals, confirming that the observed species arise exclusively from the energetic processing of HNCO ices (Figure S2). TPD profiles recorded at the photon energy of 11.00 eV revealed a distinct sublimation event at $m/z = 86$ peaking at 220 K (Figure 4). At this photon energy, all six $\text{C}_2\text{H}_2\text{N}_2\text{O}_2$ isomers are ionizable, as their AIEs fall below this threshold: carbonisocyanatidic amide (1, 10.39 eV), carbonimidisocyanatidic acid (2, 9.94 eV), 2-carbamoyl-isocyanate (3, 9.35 eV), 1,3-diazetidene-2,4-dione (4, 10.79 eV), 4-imino-1,3-oxazetidin-2-one (5, 10.55 eV), and 1,3-dioxetane-2,4-diimine (6, 10.75 eV) (Figure 2 and Table S2). When the photon energy was reduced to 10.50 eV, 4 (10.79 eV), 5 (10.55 eV), and 6 (10.75 eV) are not expected to be ionized; however, the sublimation signal persists with a consistent peak shape. This observation strongly disfavors isomers 4 and 6 and, together with the measured photoionization efficiency (PIE) onset, disfavors isomer 5 as the carrier. The signal vanished entirely at 10.20 eV, indicating that the ionization energy of the molecule lies between 10.20 and 10.50 eV. Among the candidate isomers, only carbonisocyanatidic amide has an AIE consistent with this window, enabling a confident assignment of the sublimation feature at $m/z = 86$ to carbonisocyanatidic amide.

As additional evidence for our isomer assignment, we examined the photoionization dissociation pathways of the four $\text{C}_2\text{H}_2\text{N}_2\text{O}_2$ isomers with AIEs above 10.20 eV. In this process, a single photon ionizes the neutral molecule and supplies excess energy to fragment the resulting cation.³² Quantum chemical calculations predict that the cations of isomers 1, 4, 5, and 6 have minimum dissociation thresholds of 11.49, 13.33, 12.39, and 13.97 eV, respectively (Figure 5 and Figure S3). We strategically selected 12.20 eV photons, which exceed the AIEs of all candidate isomers but lie below the dissociation thresholds of isomers 4, 5, and 6, enabling selective fragmentation of carbonisocyanatidic amide. We detected fragment ions at $m/z = 44$ whose desorption profile closely mirrored that of parent ions at $m/z = 86$ after scaling, supporting their formation during dissociative photoionization rather than a preexisting species in the ice. This observation aligns with the lowest-energy dissociation channel predicted for the carbonisocyanatidic amide cation: the cleavage of the C–N bond to produce H_2NCO^+ ($m/z = 44$) and an isocyanato radical (NCO). The cations of isomers 4, 5, and 6 each have distinct fragmentation pathways, which remain inaccessible at 12.20 eV. Consequently, the TPD signals at $m/z = 44$ are most consistent with dissociative photoionization of carbonisocyanatidic amide. The parallel desorption of parent and fragment ions, together with the theoretically predicted ionization energies, supports the formation of carbonisocyanatidic amide.

To further identify products and constrain the associated radical mechanism, we performed PIE scans, which record the ion signal intensity as a function of photon energy at selected m/z values for subliming species in the irradiated HNCO ices (Figure 6).^{31,33,34} Experiments were carried out across three temperature windows, all of which were selected based on the desorption temperature range of the corresponding species. For $m/z = 45$ (H_3NCO^+) and $m/z = 86$ ($\text{H}_2\text{N}_2\text{C}_2\text{O}_2^+$), photoionization spectra were recorded between 200 and 230 K using 0.10 eV energy steps over the 9.50–11.00 eV range. Data for $m/z = 60$ ($\text{H}_4\text{N}_2\text{CO}^+$) were acquired at 245–275 K under the same scanning conditions. A high-resolution scan (0.05

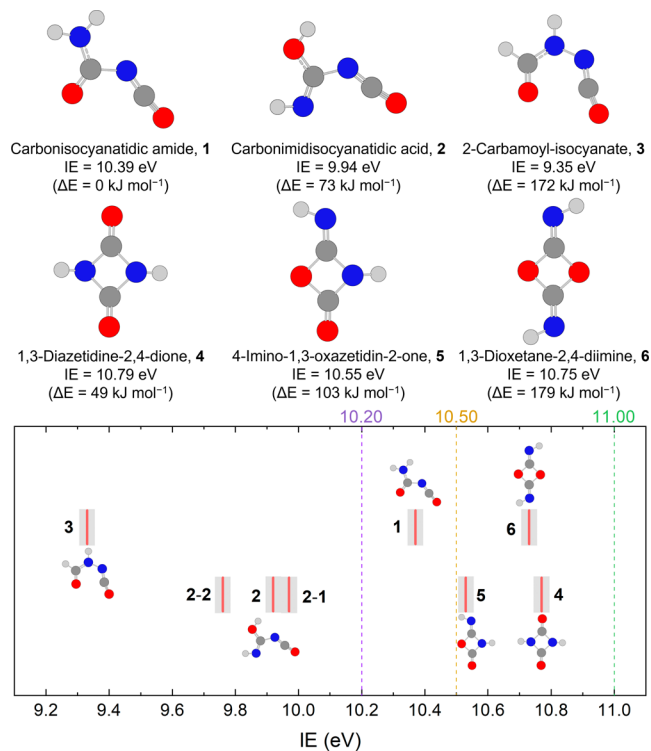


Figure 2. Computed adiabatic ionization energies (AIEs), relative energies (ΔE), and AIE ranges after error analysis for $\text{C}_2\text{H}_2\text{N}_2\text{O}_2$ isomers at the CCSD(T)/CBS// ω B97XD/aug-cc-pVTZ level of theory are shown in the upper panel. The lower panel compiles the AIEs (red solid line) corrected for the Stark effect (-0.02 eV), with the associated error ranges indicated by the shaded gray area (Table S2). The dashed vertical lines represent the vacuum ultraviolet (VUV) photon energies (11.00, 10.50, and 10.20 eV) employed for the photoionization of sublimed molecules in the gas phase. Note that 2-1 and 2-2 represent two other conformers of isomer 2.

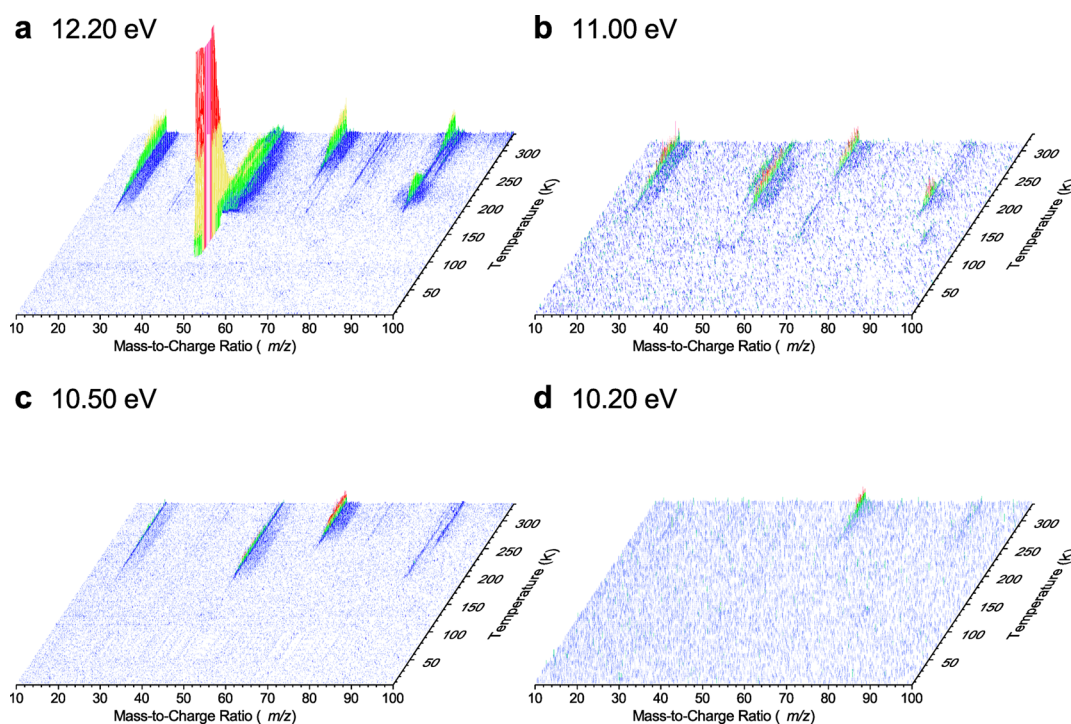
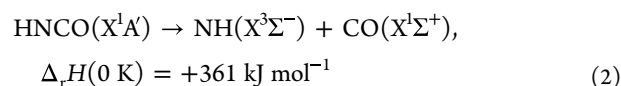
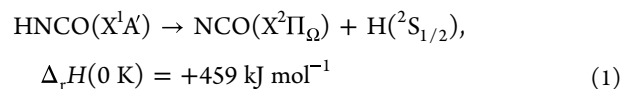


Figure 3. Synchrotron vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry (SVUV-PI-ReToF-MS) data were recorded during the temperature-programmed desorption (TPD) phase of irradiated HNCO ices at photon energies of (a) 12.20 eV, (b) 11.00 eV, (c) 10.50 eV, and (d) 10.20 eV, respectively.

eV) of $m/z = 43$ (HNCO^+) was collected between 11.40 and 12.60 eV at 122–144 K. The resulting ionization onsets for $m/z = 43, 45, 60$, and 86 were determined to be 11.600 ± 0.025 , 10.20 ± 0.05 , 9.80 ± 0.05 , and 10.40 ± 0.05 eV, respectively. All measured onsets are consistent with literature ionization energies within experimental precision: $m/z = 43$ with HNCO (11.595 ± 0.005 eV),⁴⁵ $m/z = 45$ with H_2NCHO (10.220 ± 0.005 eV),⁴⁶ and $m/z = 60$ with $\text{H}_2\text{NC(O)NH}_2$ (9.85 ± 0.05 eV).⁴⁷ Our quantum chemical calculations for carbon-isocyanatidic amide (10.39 eV) agree with the $m/z = 86$ onset within 0.01 eV. Importantly, the full PIE spectral profiles (not merely their onsets) are consistent, after normalization, with our gas-phase HNCO sample calibration PIEs, literature spectra for H_2NCHO and $\text{H}_2\text{NC(O)NH}_2$,^{46,47} and our computed curve of $\text{H}_2\text{NC(O)NCO}$ (Table S7), supporting the product assignments.

Having provided evidence for the formation of carbon-isocyanatidic amide in the irradiated HNCO ices, we now consider its plausible formation pathways. Electron irradiation of condensed HNCO initiates a complex nonequilibrium reaction network. The 5 keV kinetic energy of the incident electrons is dissipated through multiple excitation and ionization events and through secondary-electron cascades, rather than being deposited into a single HNCO molecule. Reactions 1–10 should therefore be regarded as a minimal, product-constrained network rather than an exhaustive description of the irradiation chemistry. Among the accessible primary channels, dissociation of HNCO can produce $\text{H} + \text{NCO}$ and $\text{NH} + \text{CO}$ through reactions 1 and 2, respectively. The formation of imidogen radicals (NH) and NCO fragments by electron impact has been demonstrated experimentally,⁴⁸ while the $\text{H} + \text{NCO}$ and $\text{NH} + \text{CO}$ channels and subsequent formation of carbamoyl radical (H_2NCO) have also been identified in matrix-isolation studies.⁴³ Additional neutral,

ionic, and electronically excited fragments may be generated through further dissociation and ionization, followed by electron attachment, hydrogen transfer, ion–molecule reactions, and recombination within the ice cage. The formation of CO , CO_2 , OCN^- , and tentatively formyl radical (HCO) in the FTIR difference spectrum is consistent with such a broader reaction network. Within this network, NH can capture a hydrogen atom to form amino radical (NH_2) through reaction 3, whereas the carbamoyl radical H_2NCO can be produced through H addition to HNCO or through the reaction of NH_2 with CO , as represented by reactions 4 and 5.²⁶ The identification of formamide (H_2NCHO) and urea ($\text{H}_2\text{NC(O)NH}_2$) provides indirect evidence for the involvement of these radical intermediates.^{25,26,28,29} Formamide can be formed through reactions 6–8, while recombination of H_2NCO with NH_2 provides a pathway to urea through reaction 9.^{49,50} Carbonisocyanatidic amide may be formed most directly through the highly exoergic radical–radical recombination of H_2NCO with NCO in reaction 10. However, stepwise radical–molecule addition and association or recombination involving excited or ionized HNCO species cannot be excluded. Reaction 10 is therefore proposed as a chemically direct pathway consistent with the observed products and calculated thermochemistry, rather than as a uniquely established mechanism.



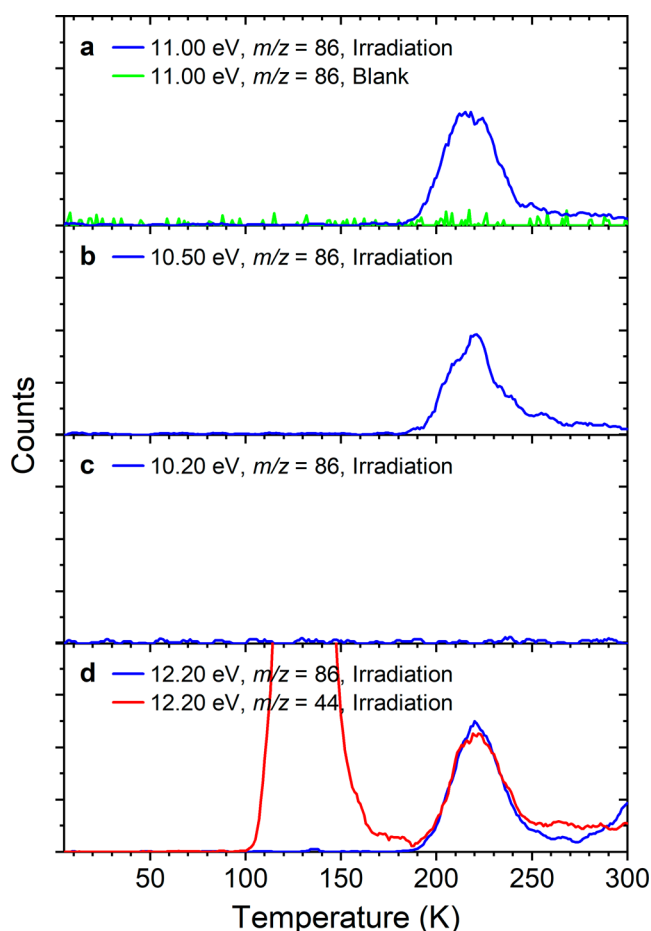
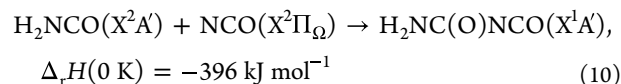
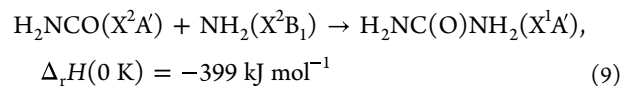
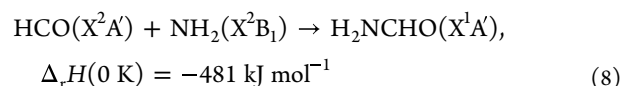
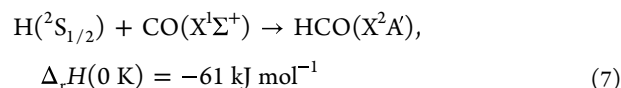
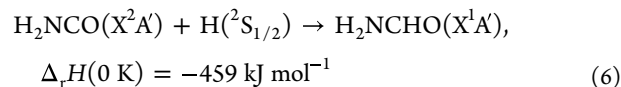
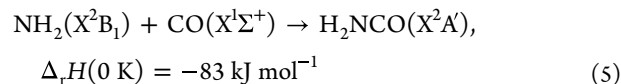
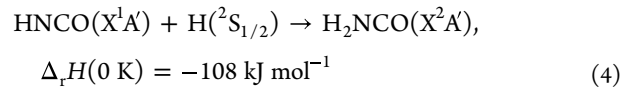
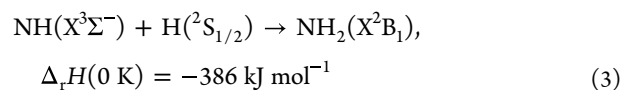


Figure 4. TPD sublimation profiles of irradiated and nonirradiated (blank experiment) HNCO ices at photon energies of (a) 11.00 eV, (b) 10.50 eV, (c) 10.20 eV, and (d) 12.20 eV, respectively.



Thermodynamically, the reaction energy for the conversion of two HNCO molecules to carbonisocyanatidic amide is exoergic, with a total reaction energy ($\Delta_r H$ at 0 K) of -45 kJ mol^{-1} . This exoergicity indicates that the overall transformation is thermodynamically allowed once reactive radicals are generated, although its kinetic accessibility depends on

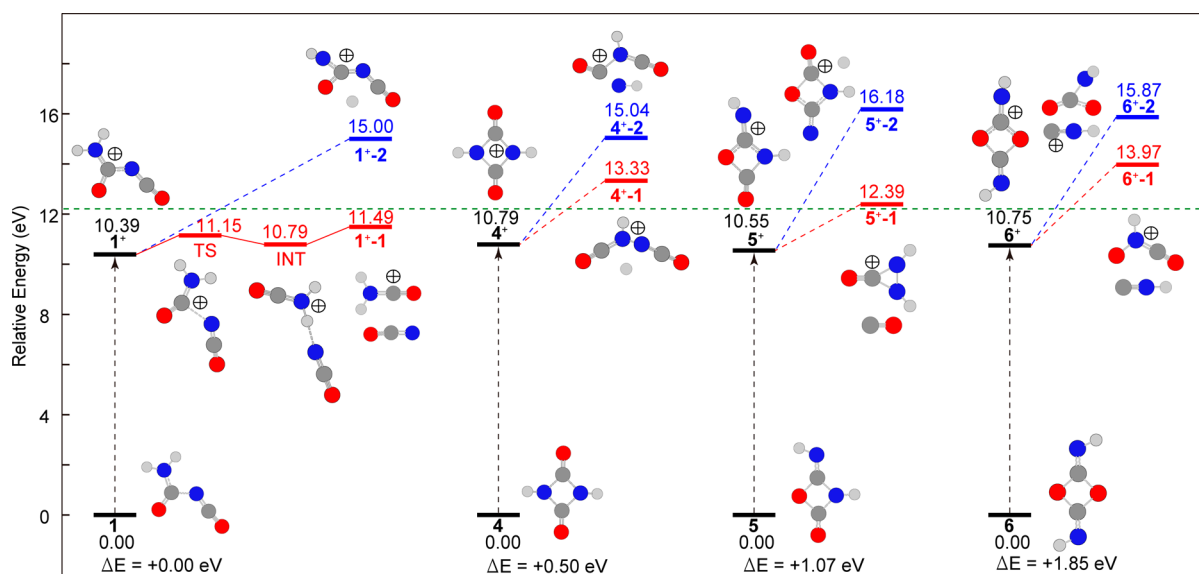


Figure 5. Calculated photoionization and cation-dissociation energy profiles of isomers 1, 4, 5, and 6. The neutral ground state of each isomer is independently set to 0.00 eV, and all energies within each profile are referenced to this local zero. On a common energy scale referenced to neutral isomer 1, the relative energies (ΔE) of neutral isomers 1, 4, 5, and 6 are 0.00, 0.50, 1.07, and 1.85 eV, respectively. Accordingly, energies on this common scale can be obtained by adding the corresponding neutral-isomer offset to each value shown in the respective profile. Dashed vertical arrows indicate the corresponding adiabatic ionization energies (AIEs). Red and blue lines depict the calculated cation-dissociation pathways, while the green dashed line marks the experimental photon energy of 12.20 eV relative to the neutral ground state of each isomer.

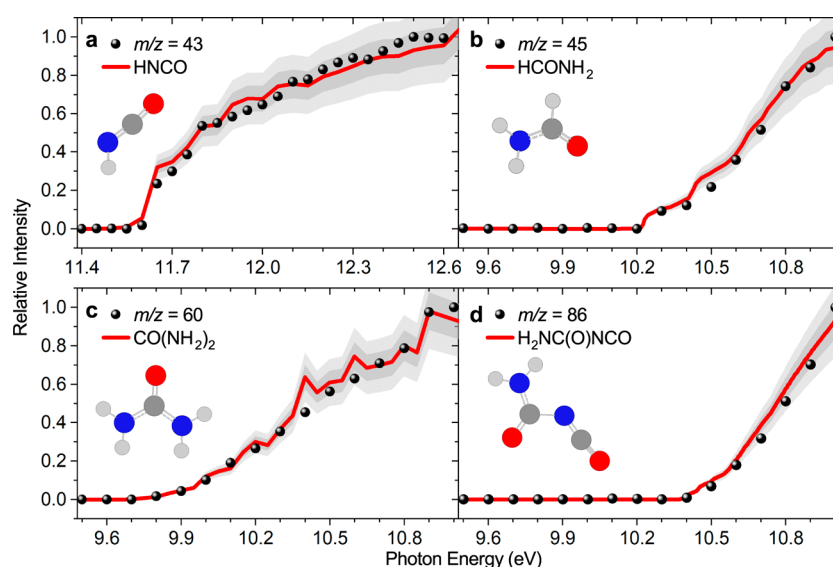


Figure 6. Photoionization efficiency (PIE) curves for the species linked to (a) $m/z = 43$, (b) $m/z = 45$, (c) $m/z = 60$, and (d) $m/z = 86$. The circles represent experimental data, while the red lines indicate fits to the reference or calculated PIE curves. The uncertainties in the fit are noted with dark-gray (1σ) and light-gray (2σ) shaded regions.

irradiation-induced radical production and recombination. Thus, carbonisocyanatidic amide should not be viewed simply as a terminal product, but as a reactive intermediate that may participate in further molecular growth. As illustrated in Figure 1, the structural motif of carbonisocyanatidic amide contains a N–C–O connectivity related to pyrimidine precursors. However, no reaction of carbonisocyanatidic amide with unsaturated hydrocarbons has yet been demonstrated under astrophysically relevant conditions. Acetylene (C_2H_2) and methylacetylene (C_3H_4) are logical candidates for future studies because their $C\equiv C$ units could, in principle, provide the C5–C6 segment required for pyrimidine-ring closure; methylacetylene could additionally supply the C5 methyl substituent of thymine. Although synthetic alkyne–isocyanate cyclizations provide chemical precedent for this proposal, they do not establish that an analogous reaction involving carbonisocyanatidic amide is kinetically accessible in low-temperature interstellar ices or in the gas phase. Targeted experiments and reaction-pathway calculations are therefore needed to determine whether such chemistry can contribute to the formation of uracil or thymine under astrophysical conditions.

Our findings demonstrate that carbonisocyanatidic amide can be produced in pure HNCO ice through a radical–radical mechanism initiated by energetic-electron irradiation, providing a laboratory analogue for chemistry driven by GCR-generated secondary electrons in interstellar ices. The corresponding energy deposition translates to reaction time scales of about 1.5×10^7 years in dense molecular clouds, comparable to their typical lifetimes. As protostellar systems evolve, thermal sublimation during the warm-up phase releases these molecules into the gas phase, potentially making them detectable by ALMA in protostellar envelopes and hot corinos, provided that laboratory rotational spectra become available. Carbonisocyanatidic amide is therefore best regarded as a structurally relevant candidate intermediate, rather than a demonstrated direct precursor to uracil or thymine, for future studies of pyrimidine nucleobase chemistry. During solar system formation, carbonisocyanatidic amide and its deriva-

tives could be sequestered within planetoids, comets, and asteroids, ultimately reaching the prebiotic Earth through impact delivery. This exogenous input hypothesis is supported by recent analyses of samples returned from the carbonaceous asteroids Bennu and Ryugu, and in the Murchison meteorite, both of which revealed extraterrestrial nucleobases including uracil and thymine.^{8–11}

In conclusion, our study presents experimental evidence for the bottom-up abiotic formation of carbonisocyanatidic amide in low-temperature HNCO ices subjected to energetic electrons. By employing SVUV-PI-ReToF-MS and PIE curve analysis, we achieve isomer-specific identification, further supported by quantum chemical calculations. Our results address a critical gap in our understanding of interstellar nitrogen–carbon–oxygen chemistry by identifying a pyrimidine-relevant intermediate formed in HNCO ice (Figure 1). By establishing carbonisocyanatidic amide as a candidate astrochemical intermediate, we identify a testable target for studies of how simple nitrogen-bearing species might evolve toward molecular frameworks relevant to pyrimidine nucleobases. This discovery not only motivates tests of proposed reaction pathways but also identifies carbonisocyanatidic amide as a promising astrochemical target for future telescopic observations and sample-return missions.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.jpclett.6c02249>.

Experimental and computational methods, FTIR spectra and their assessments, SVUV-PI-ReToF-MS data, calculated potential dissociation channels and corresponding dissociation energies for the parent cations of isomers 4–6, interference pattern observed during deposition of HNCO ices, CASINO simulation of the electron penetration, EI-QMS-TPD data, relative energies, and error analysis of $C_2H_2N_2O_2$ isomers, detected ion signals and proposed assignments in irradiated HNCO ices, experimental conditions, average dose

calculation, geometries, energies, and frequencies of neutral species, cations, and dissociative channels for C₂H₂N₂O₂ isomers, Franck–Condon factors (FCFs) of carbonisocyanatidic amide (PDF)

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