Product Channels in the 193-nm Photodissociation of HCNO (Fulminic Acid)

Wenhui Feng¹ and John F. Hershberger^{*}

*Department of Chemistry and Biochemistry, Dept. 2735, PO Box 6050,
North Dakota State University, Fargo, ND 58108-6050*

Abstract

IR diode laser spectroscopy was used to detect the products of HCNO (fulminic acid) photolysis at 193 nm. Six product channels are energetically possible at this photolysis wavelength: O + HCN, H + NCO/CNO, CN + OH, CO + NH, NO + CH and HNCO. In some experiments, isotopically labeled ¹⁵N¹⁸O, C₂D₆ or C₆H₁₂ reagents were included into the photolysis mixture in order to suppress and/or redirect possible secondary reactions. HCN, OC¹⁸O, ¹⁵N¹⁵NO, CO, DCN and HNCO molecules were detected upon laser photolysis of HCNO/reagents/buffer gas mixtures. Analysis of the yields of product molecules leads to the following photolysis quantum yields: ϕ_{1a} (O+HCN) = 0.38 ± 0.04 , ϕ_{1b} (H + (NCO)) = 0.07 ± 0.02 , ϕ_{1c} (CN + OH) = 0.24 ± 0.03 , ϕ_{1d} (CO + NH(a¹Δ)) < 0.22 ± 0.1 , ϕ_{1e} (HNCO) = 0.02 ± 0.01 and ϕ_{1f} (CH + NO) = 0.21 ± 0.1 , respectively.

Key words: laser spectroscopy, fulminic acid, photodissociation, photolysis quantum yield

I made correction at P1, P4, P10, P14, P15, changing fig 2 and 3 ordering according to the text.

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^{*} Corresponding author. Email: john.hershberger@ndsu.edu. FAX (701)-231-8831

1. Introduction

Fulminic acid (HCNO) and isocyanic acid (HNCO) are important intermediates in NO-reburning processes for reduction of NO_x pollutants from fossil-fuel combustion emission [1] and have also been found existing in a large variety of environments in the interstellar medium [2]. HCNO (fulminic acid) is the less stable isomer of isocyanic acid; the kinetics of several reactions involving HCNO has only recently been studied [3-7]. There is only one previous study of the photochemistry of HCNO, an infrared laser spectroscopic study from our laboratory that identified five separate photolysis channels in the 248 nm photodissociation of this molecule [8].

In this paper, we extend the previous study to include photolysis at 193 nm. At this wavelength, an additional channel (1f) becomes energetically accessible, resulting in six possible channels:

NCO is written as (NCO) to indicate that we cannot distinguish between NCO and CNO isomers in this study, because we detect secondary products of NCO (or CNO) reactions, rather than the NCO radical itself. Figure 1 shows the energetics of these species. The thermochemical information has been obtained from standard tables [9] as well as other literature for the heats of formation of NCO [10] and NH (*a*¹Δ) [11]. Formation of ground state NH (*X*³Σ⁻) is also possible, but is less likely as it is a spin-forbidden process.

Figure 1 Relative energy levels of possible photolysis products of HCNO photolysis. Thresholds (kJ/mol) compared to HCNO: -291.2 (HNCO), 95.1 (CO + NH (X³Σ⁻)), 174.5 (H + NCO), 213.3 (O + HCN), 261.9 (CO + NH (a¹Δ)), 303.1 (OH + CN), 436.6 (H + CNO), 516.1 (CH + NO), 620 (193 nm photon) and 482.6 (248 nm photo).

2. Experimental Section

The experimental apparatus was described in our previous study [8]. Briefly, HCNO was photolyzed by 193 nm light from an excimer laser (Coherent, Compex-pro). Reaction products were detected by transient infrared diode laser absorption spectroscopy using lead salts diode lasers (Laser Components) operating in the 80-110 K temperature range. Transient infrared absorption signals were recorded on a digital oscilloscope (Lecroy, Wavesurfer 422) and transferred to a computer for analysis. All experiments were performed at 298 K.

HCNO samples were synthesized as previously described [8,12-14]^{1,2,3} by flash vacuum pyrolysis of 3-phenyl-4-oximino-isoxazol-5(4H)-one. Sample purity was characterized by FT-IR spectroscopy via a strong HCNO absorption band at 2195 cm⁻¹ [15], and a strong HNCO band at 2168 cm⁻¹ [16]. The sample purity was estimated at 95% or better, with only small CO₂ and HNCO impurities. Samples were kept at 77 K except when filling the reaction cell.

CF₄ and SF₆ (Matheson) was purified by repeated freeze-pump-thaw cycles at 77 K and by passing through an Ascarite II column to remove traces of CO₂. ¹⁵N¹⁸O (Isotec) was purified

by repeated freeze-pump-thaw cycles at 153 K. The following molecules were probed using infrared diode laser absorption spectroscopy:

HCN ($v=1 \leftarrow v=0$)	P(17) at 3258.441 cm^{-1}
DCN ($v=1 \leftarrow v=0$)	R(7) at 2648.9 cm^{-1}
OC ¹⁸ O ($v_1, v=1 \leftarrow v=0$)	P(15) at 2320.46 cm^{-1}
HNCO ($v=1 \leftarrow v=0$)	R(10) at 2276.71 cm^{-1}
¹⁵ N ₂ O ($v=1 \leftarrow v=0$)	P(5) at 2150.62 cm^{-1}
CO ($v=1 \leftarrow v=0$)	P(6) at 2119.68 cm^{-1}

The HITRAN molecular database was used to locate and identify the spectral lines of OC¹⁸O and HCN product molecules [17]. Other published spectral data were used to locate and identify DCN [18], ¹⁵N₂O [19] and HNCO [16] lines.

Typical experimental conditions were P(HCNO) = 0.1 Torr, P(¹⁵N¹⁸O) = P(¹⁵N¹⁶O) = 1.0 Torr, P(SF₆) = P(CF₄) = 1.50 Torr, P(C₂D₆) = 0.5 - 7.0 Torr, P(C₆H₁₂, cyclohexane) = 0.5 - 3.0 Torr and 193 nm laser pulse energies of 8.5 mJ (fluence of ~30 mJ/cm²). In order to minimize waste of HCNO samples, all experiments were performed using static gas fills. Typical transient signals were signal averaged over only four photolysis laser shots, after which the gas cell was evacuated and refilled for further experiments. This procedure minimizes any buildup of photolysis products, and therefore minimizes effects of secondary photolysis. No dependence of signal amplitudes on the number of photolysis laser shots was observed.

3. Results

Infrared diode laser absorption was used to detect product molecules (or products of secondary chemistry) from channel 1a - 1f upon 248 nm laser photolysis of HCNO/ buffer gas. In order to modify and/or suppress potential secondary chemistry, additional reagents were sometimes included in the reaction mixture, as described below. Figure 2 shows two typical signals for detection of HCN and CO₂ molecules. The purpose of the isotopic labelling will be discussed in section 3.2, below. Typically, transient signals show a fast (~10-100 μsec) rise, followed by a slow (~1 msec) decay. The rise is attributed to formation of the detected product by either direct photolysis and/or subsequent secondary chemistry, as described below. The

decay is attributed to diffusion of molecules out of the probed volume. The rate of the rise is primarily determined by the rate of collisional relaxation of a nascent vibrational distribution to a Boltzmann distribution. The buffer gas (CF₄ or SF₆) [4,5] was used to maximize this relaxation rate. Our product yield measurements assume that the detected products have reached a Boltzmann distribution of internal states on the 10 - 100 μ s timescale of the transient signals.

In order to estimate the yields, the slow decay portion of each transient signal was fit to a single exponential decay function. Transient signal amplitudes were obtained by extrapolation to $t = 0$ (this extrapolated amplitude was typically a small (~5-15%) increase compared to the peak-peak amplitudes). Because the correction vs. the peak-peak amplitude is small, and about the same for different detected molecules, errors in this procedure due to the fact that diffusion out of a cylindrical volume is not strictly exponential are insignificant.

The resulting amplitudes were converted into absolute concentrations using HITRAN line strengths for all of the detected molecules except for DCN molecules, which were calibrated. Table 1 shows the resulting yields of the detected molecules.

Our previous studies [2-6] show that HCNO is a highly reactive molecule. Many secondary reactions following the photolysis can therefore occur. Most but not all of this secondary chemistry is identical to that considered in our previous study [8]:

Reactions (2)-(6) have been studied previously in our lab [2-6], resulting in the following rate constants: $k_2 = (5.32 \pm 0.4) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_3 = (1.04 \pm 0.1) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_4 = (1.58 \pm 0.2) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, $k_5 = (3.4 \pm 0.3) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_6 \leq 2.1 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K. While the rate of $H + HCNO$, reaction (7), is not

experimentally known, our previous study [8] showed that it was too slow to affect the results of HCNO photolysis experiments. Reactions (2)-(5) are fast and may produce some of the same product molecules as those probed in these experiments, potentially complicating the interpretation of product yields. The approach used here is similar to that used previously [8], in which we include additional reagents in the reaction mixture in order to suppress or redirect these secondary reactions, as described in detail below.

Figure 2 Transient signals of HCN and $^{16}\text{O}^{18}\text{O}$ detected upon laser photolysis of HCNO (0.1 Torr)/ $^{15}\text{N}^{18}\text{O}$ (1 Torr)/ SF_6 (1.5 Torr) mixture.

Table 1: Raw Product Yields^a

Product	Yield (in units of 10^{12} molecule cm^{-3})
HCN	17.9 ± 1.8
OC^{18}O	1.8 ± 0.1
DCN	11.1 ± 1.2
CO	$<10.3 \pm 2.0$
HNCO	1.0 ± 0.2
$^{15}\text{N}_2\text{O}$	9.3 ± 0.7

^a Experimental conditions: P (HCNO) = 0.1 Torr, P($^{15}\text{N}^{18}\text{O}$) = P($^{15}\text{N}^{16}\text{O}$) = 1.0 Torr, P (SF_6) = 1.5 Torr (for HCN, NCO and DCN detection), P (CF_4) = 1.5 Torr (for CO detection only), 193 nm photolysis laser pulse energy ~ 8.5 mJ. Uncertainties represent one standard deviation.

Some additional secondary chemistry, potentially present in this study but not relevant to our previous study, is due to the possible presence of channel (1f), forming CH + NO photoproducts. This channel was not energetically accessible at 248 nm, but is at 193 nm. If this channel is active, the following reaction must be considered:

The rate constant of reaction (8) is unknown, but CH is a highly reactive species, so it is likely that this reaction is fast. Products are also unknown, but likely include many of the same molecules probed in these experiments.

3.1 Product channel (1f), CH+NO

The most obvious approach to quantifying this channel would be to directly detect and quantify the yield of NO products. This approach is complicated, however, by secondary sources of NO, including reaction (2), (3), (4), (5c), etc. We therefore used an alternative approach to detect this channel: we included an excess of $^{15}\text{N}^{16}\text{O}$ in the reaction mixture: HCNO (0.1

Torr)/ $^{15}\text{N}^{16}\text{O}$ (1.0 Torr)/ SF_6 (1.5 Torr). Under these conditions, any CH radicals produced in (1f) will react with $^{15}\text{N}^{16}\text{O}$ as follows:

The product branching ratio of reaction has been estimated to be $\phi_{9a} = 0.21 \pm 0.1$; $\phi_{9b} = 0.72 \pm 0.1$ [20]. A subsequent secondary reaction then produces $^{15}\text{N}^{15}\text{NO}$:

(Product branching ratios at 296 K: $\phi_{10a} = 0.44 \pm 0.07$; $\phi_{10b} = 0.56 \pm 0.07$) [21-22].

We then detected the double labeled $^{15}\text{N}^{15}\text{NO}$ molecule, using spectral line positions reported previously [19]. Although the branching ratio into (9a) is modest, N_2O is a very strong infrared absorber, so this experiment has a reasonably low detection limit. We found a small transient signal attributable to $^{15}\text{N}^{15}\text{NO}$, shown in Figure 3.

Figure 3 The $^{15}\text{N}^{15}\text{NO}$ transient IR absorption signal detected upon photolysis of HCNO (0.1 Torr)/ $^{15}\text{N}^{16}\text{O}$ (1.0 Torr)/ SF_6 (1.5 Torr).

3.2 Product channel (1a), O + HCN

The procedure for quantification of channel (1a) is similar to that described previously [8]. We directly detect the HCN photolysis product by transient absorption, as shown in Figure 2 (top panel). The HCN yield from photolysis of HCNO could arise from channel (1a), but also may have contributions from reaction (4) if channel (1b) is significant. By including an excess of isotopically labeled $^{15}\text{N}^{18}\text{O}$ reagent, however, reaction (4) is suppressed:

Where $\phi_{10a} = 0.44$ and $\phi_{10b} = 0.56$ [21-22], and $k_{10} = (4.3 \pm 0.4) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ [6]. Based on the rate constant of (4) and (10), we estimate that a 10:1 ratio of $^{15}\text{N}^{18}\text{O}$ to HCNO is sufficient to ensure that nearly all NCO radicals react by (10) rather than (4), and therefore do not result in HCN production. Reaction (10) will not suppress reaction (3), $\text{CN} + \text{HCNO}$, because the $\text{CN} + \text{NO}$ reaction is slow at the low pressures used in these experiments. Reaction (3) produces HCCN radicals [4,7] which then react with $^{15}\text{N}^{18}\text{O}$, producing labeled HC^{15}N molecules:

In these experiments, however, we detect the non-labeled HC^{14}N isotope, which is not affected by this secondary chemistry. The nitrogen-15 labeling is therefore important for this experiment (the oxygen-18 labeling is not). We also note that any CH formed from channel (1f) will react with $^{15}\text{N}^{18}\text{O}$, effectively suppressing reaction (8). Although $\text{CH} + \text{NO}$ produces HCN as a product, $\text{CH} + {}^{15}\text{N}^{18}\text{O}$ would make HC^{15}N , not the detected HC^{14}N molecule.

Other potential secondary reactions, such as $\text{O} + \text{HCNO}$, $\text{OH} + \text{HCNO}$, $\text{NH} + \text{NO}$, and $\text{NH} + \text{HCNO}$ do not produce significant amounts of HCN. Therefore, we can confidently

attribute the HCN signal obtained upon photolysis of a HCNO (0.1 Torr)/ $^{15}\text{N}^{18}\text{O}$ (1.0 Torr)/ SF_6 (1.5 Torr) mixture, as shown in Figure 2, to photolysis channel (1a).

3.3 Product channel (1b), $\text{H} + (\text{NCO})$

We assume here, as in our previous study [8] that if the high energy CNO isomer is formed, it quickly converts to the more stable NCO; as a result we do not distinguish between NCO and CNO. In order to quantify the yield of this channel, we added isotopically labeled $^{15}\text{N}^{18}\text{O}$ reagent in the photolysis mixture as described above (section 3.2), resulting in reaction (10), to produce OC^{18}O . A transient signal is shown in Figure 2 (bottom panel). (In this experiment, the oxygen-18 labeling is crucial, while the nitrogen-15 labeling is not). Assuming an excess of $^{15}\text{N}^{18}\text{O}$, resulting in most NCO radicals reacting via (10), and knowing the branching ratio of $\phi_{10b} = 0.56$, we quantify the yield of NCO molecules originally produced in photolysis channel (1b):

$$[\text{NCO}]_{1b} = [\text{OC}^{18}\text{O}] / 0.56$$

Additional secondary chemistry that can also produce CO_2 includes

The notation (10b*) is used to identify an isotopic variant of reaction (10b). CO_2 molecules in reaction (10b*) are double labeled ($^{18}\text{OC}^{18}\text{O}$) and do not contribute to the yield of the detected OC^{18}O . A similar argument can be made for secondary chemistry involving CH radicals: reactions (9a) and (10b), when using $^{15}\text{N}^{18}\text{O}$, would also produce $^{18}\text{OC}^{18}\text{O}$, not the detected OC^{18}O .

3.4 Product channel (1c), CN + OH

In our previous publication [8], several approaches were used to quantify the CN+OH channel. The most effective method proved to be the addition of deuterated ethane, C₂D₆, resulting production of DCN:

This approach was used in the present experiments. Figure 4 shows the resulting transient signal for DCN. We measured these DCN signals as a function of C₂D₆ pressure upon photolysis of HCNO (0.1Torr)/C₂D₆ (variable: 0.5-7.0 Torr)/SF₆ (1.5 Torr) mixtures. These data, after calibration by a procedure described previously [8], which includes a modest correction for pressure broadening effects, are shown in Figure 5.

Figure 4 Transient signal of DCN detected upon photolysis of HCNO(0.1Torr)/C₂D₆ (5.0 Torr) / SF₆ (1.5 Torr) mixture.

Figure 5 The yields of DCN as the function C_2D_6 pressures. DCN was detected upon photolysis of HCNO (0.1 Torr)/ C_2D_6 (variable: 0-7.0 Torr)/ SF_6 (1.5 Torr) mixture; 193 nm photolysis laser pulse energy ~ 8.5 mJ. The experimental data were simulated by an function:

$$y = 34.1 - 28.5e^{-(x+3.0)/152.8} - 840.2e^{-(x+3.0)/0.6} - 908.1e^{-(x+3.0)/0.6}$$

As shown in Figure 5, the DCN yield has not become completely constant even at the highest C_2D_6 pressures used. As discussed previously [8], this is roughly consistent with the relevant kinetics; $k_{12} \sim 1.2 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ [8], and $k_3 = (1.04 \pm 0.1) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ [4]. Based on the rate constants involved, we estimate that about 30 Torr of C_2D_6 is needed for reaction (12) to suppress most of reaction (3). The data was therefore fit to an empirical three parameter exponential equation, as shown in Figure 5. Extrapolating this equation, we estimate $[DCN] = (1.11 \pm 0.12) \times 10^{13} \text{ molecule cm}^{-3}$ at $[C_2D_6] = 30$ Torr. This result is shown in Table 2.

3.5 Product channel (1d), CO + NH

We investigated the channel by direct detection of CO. If an excess of a hydrocarbon molecule such as C_6H_{12} (cyclohexane) is included, most of the secondary chemistry of radicals reacting with HCNO is suppressed, as follows:

Figure 6 shows the CO yield obtained upon 193-nm photolysis of HCNO in the presence of C_6H_{12} . As shown, the yield drops as the C_6H_{12} pressure is increased, indicating that reactions (13) - (16) do in fact suppress much of the secondary chemistry, reactions (2) - (5). At about 2 - 3 Torr of C_6H_{12} , the CO yield has reached an approximately constant value. By comparing the rate constants of (13) - (16) with those of (2) - (5), we estimate that this cyclohexane pressure is sufficient to suppress most of reactions (2), (3), and (5), but probably only partially suppressed reaction (4), because reaction (16) is relatively slow. We therefore must interpret the limiting CO yield in Figure 6 as an estimate of the upper limit to the yield of channel (1d).

Figure 6 The CO yield as the function of the added C_6H_{12} concentration. Transient signal of CO radical detected upon photolysis of HCNO (0.1 Torr)/ C_6H_{12} (cyclohexane, variable pressure)/ CF_4 (1.5 Torr) mixture.

3.6 Product channel (1e), HNCO

As shown in Figure 7, a small absorption transient was detected for HNCO, the result of photoisomerization. This signal (peak amplitudes) was converted to an absolute concentration using the calibration procedure described previously [8]. This measurement is subject to significant uncertainties that are described in detail in our previous study [8], but we do estimate a very small yield of channel (1e).

Figure 7 The HNCO transient IR absorption signal detected upon photolysis of HCNO (0.1 Torr)/SF₆ (1.5 Torr) using the R(10) line of HNCO. The brief negative spike at t=0 is an artifact due to a small HNCO impurity present in the mixture.

3.7 Summary of Quantum Yields

Table 1, as described above, shows the raw yields of the detected molecules. Table 2 shows the resulting yields of the six HCNO photolysis channels after the above analysis to account for secondary chemistry. The sum of the channels gives a total product yield of 4.3×10^{13} molecule cm⁻³. We then converted the product yields into photolysis quantum yields, using a

measured value of the UV absorption coefficient of HCNO at 193 nm: $\alpha_{193} = (1.83 \pm 0.16) \times 10^{-2}$ Torr⁻¹cm⁻¹, equivalent to a cross section of $\sigma_{193} = (5.65 \pm 0.48) \times 10^{-19}$ cm² molecule⁻¹. Under the experimental conditions of Table 2, we estimate the number density of absorbed photons to be 4.69×10^{13} molecule cm⁻³. We then determined the quantum yields, as shown in Table 3. The sum of the quantum yields is 0.92 – 1.14, depending on the value used for the NH + CO channel. The uncertainties quoted in Table 3 include random errors (1 σ) inherent in the measurements as well as consideration of systematic errors, primarily due to estimated uncertainties in the infrared linestrengths and HCNO UV absorption coefficient. The yield of NH + CO is expressed as an upper limit, as described above.

It is worthwhile to compare our current results at 193-nm with the previously obtained 248-nm photolysis yields. As shown in Table 3, multiple channels are present at both photolysis wavelengths, although channel (1e) is sufficiently minor to be considered negligible. At both wavelengths, O + HCN is the most important photolysis channel. The primary difference between the two wavelengths is that channel (1b), H + (NCO), is much less prevalent at 193 nm than at 248 nm, while channel (1f), which is not energetically accessible at 248 nm but is accessible and is a significant minor channel at 193 nm.

Table 2: Yields of Product Channels of HCNO Photolysis^a

Product	Yield (in units of 10^{12} molecule cm ⁻³)
HCN	17.9 ± 1.8
NCO	3.2 ± 0.2
CN	10.1 ± 1.2
CO	$<10.3 \pm 2.0$
HNCO	1.0 ± 0.2
CH	9.8 ± 0.8
Total	43.0

^a Experimental conditions are same as in Table 1

Table 3: Quantum Yields of HCNO Photolysis Products at 248 and 193nm

Product Channel	$\phi(248 \text{ nm})^a$	$\phi(193\text{nm})^b$
O + HCN	0.39 ± 0.07	0.38 ± 0.04
H + (NCO)	0.21 ± 0.04	0.07 ± 0.02
CN + OH	0.16 ± 0.04	0.24 ± 0.03
NH + CO	0.19 ± 0.03	$<0.22 \pm 0.04$
HNCO	0.05 ± 0.02	0.02 ± 0.01
CH + NO	0.00	0.21 ± 0.06
Total	1.00 ± 0.15	0.92 - 1.11

^a Results from reference [8]

^b Results from this study.

4. Conclusions

Infrared diode laser spectroscopy was used to study the photolysis products of fulminic acid (HCNO). The results show that six product channels have a measurable yield, and that O + HCN (1a) is the major but not dominant product channel. Photolysis quantum yields ϕ_{1a} (O + HCN) = 0.38 ± 0.04 , ϕ_{1b} (H + (NCO)) = 0.07 ± 0.02 , ϕ_{1c} (CN + OH) = 0.24 ± 0.03 , ϕ_{1d} (CO + NH($a^1\Delta$)) < 0.22, ϕ_{1e} (HNCO) = 0.02 ± 0.01 , ϕ_{1f} (CH + NO) = 0.21 ± 0.06 , respectively.

Acknowledgement

This work was supported by Division of Chemical Sciences, Office of Basic Energy Sciences of the Department of Energy, Grant DE-FG03-96ER14645.

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