# Kinetics of HCCl + NO<sub>x</sub> Reactions

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ABSTRACT: The kinetics of reactions of HCCl with NO and NO<sub>2</sub> were investigated over the temperature ranges 298–572 k and 298–476 k, respectively, using laser-induced fluorescence spectroscopy to measure total rate constants and time-resolved infrared diode laser absorption spectroscopy to probe reaction products. Both reactions are fast, with  $k(\text{HCCl} + \text{NO}) = (2.75 \pm 0.2) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ and } k(\text{HCCl} + \text{NO}_2) = (1.10 \pm 0.2) \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ at } 296 \text{ K}$ . Both rate constants displayed only a slight temperature dependence. Detection of products in the HCCl + NO reaction at 296 K indicates that HCNO + Cl is the major product with a branching ratio of  $\phi = 0.68 \pm 0.06$ , and NCO + HCl is a minor channel with  $\phi = 0.24 \pm 0.04$ . © 2001 John Wiley & Sons, Inc. Int J Chem Kinet 34: 12–17, 2002

# INTRODUCTION

The detailed gas-phase chemistry of nitrogen oxides is of great interest because of the role these compounds play in pollutant emissions from fossil fuel combustion [1]. Chlorinated hydrocarbons are frequently present in hazardous waste incinerator emissions [2]. The kinetics of chlorinated hydrocarbon fragments such as HCCl are therefore of interest in efforts to model these processes.

Unlike the unsubstituted carbene CH<sub>2</sub>, the ground electronic state of HCCl is a singlet. Although this species has been characterized spectroscopically [3,4], relatively little experimental data on HCCl kinetics are available. In general, HCCl is known to be moderately reactive with unsaturated hydrocarbons and NO, but unreactive with O<sub>2</sub> [5,6]. One previous study of the HCCl + NO reaction has been reported, in which a room temperature rate constant of  $(1.5 \pm 0.5) \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> was reported [5]. No rate constant for HCCl + NO<sub>2</sub> kinetics has been published, nor

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is any information on product channels available for either title reaction.

We report here kinetic studies of the reactions of HCCl ( $\tilde{X}^1A'$ ) with NO and NO<sub>2</sub>. HCCl is produced by the 193-nm excimer laser photolysis of CHClBr<sub>2</sub>. This precursor is known to produce HCCl from previous kinetic and spectroscopic studies [4–6], and cannot produce CH or CCl radicals from a single 193-nm photon. HCCl is probed by laser-induced fluorescence near 603 nm to measure total rate constants [3]. Both title reactions have several possible product channels:

$$\begin{array}{l} \mathrm{HCCl} + \mathrm{NO} \rightarrow \mathrm{HCNO} + \mathrm{Cl} \\ \Delta_{\mathrm{r}} H^0 = -129.6 \ \mathrm{kJ} \ \mathrm{mol}^{-1} \quad (1a) \end{array}$$

$$\begin{array}{l} \mathrm{HCCl} + \mathrm{NO} \rightarrow \mathrm{HNCO} + \mathrm{Cl} \\ \Delta_{\mathrm{r}} H^0 = -405.7 \ \mathrm{kJ} \ \mathrm{mol}^{-1} \quad (\mathrm{1b}) \end{array}$$

$$\begin{array}{l} \mathrm{HCCl} + \mathrm{NO} \rightarrow \mathrm{NCO} + \mathrm{HCl} \\ \Delta_{\mathrm{r}} H^{0} = -386.2 \ \mathrm{kJ} \ \mathrm{mol}^{-1} \quad (1\mathrm{c}) \end{array}$$

$$\text{HCCl} + \text{NO} \rightarrow \text{HCN} + \text{ClO}$$
  
 $\Delta_{\text{r}} H^0 = -188.9 \text{ kJ mol}^{-1}$  (1d)

HCCl + NO → CN + HOCl  

$$\Delta_{\rm r} H^0 = -64.7 \text{ kJ mol}^{-1}$$
 (1e)

$$\begin{split} \mathrm{HCCl} + \mathrm{NO}_2 &\to \mathrm{HCNO} + \mathrm{ClO} \\ \Delta_\mathrm{r} H^0 = +92.5 \ \mathrm{kJ} \ \mathrm{mol}^{-1} \end{split} \tag{2a}$$

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$$\begin{array}{l} \mathrm{HCCl} + \mathrm{NO}_2 \rightarrow \ \mathrm{HNCO} + \mathrm{ClO} \\ \Delta_\mathrm{r} H^0 = -368.5 \ \mathrm{kJ} \ \mathrm{mol}^{-1} \quad \ (2\mathrm{b}) \end{array}$$

$$\begin{aligned} \text{HCCl} + \text{NO}_2 &\to \text{NCO} + \text{HOCl} \\ \Delta_{\text{r}} H^0 &= -311.2 \text{ kJ mol}^{-1} \end{aligned} (2c)$$

$$\begin{aligned} \mathrm{HCCl} + \mathrm{NO}_2 &\to \mathrm{HCN} + \mathrm{ClO}_2 \\ \Delta_\mathrm{r} H^0 &= -128.4 \ \mathrm{kJ} \ \mathrm{mol}^{-1} \quad (\mathrm{2d}) \end{aligned}$$

Thermochemical data was taken from JANAF tables [7], except for NCO, for which  $\Delta_{\rm f} H^0 = 131.38$  kJ mol<sup>-1</sup> was used [8].

# **EXPERIMENTAL**

The photolysis laser light was provided by an excimer laser (Lambda Physik COMPEX 200) operating at 193 nm. Typical photolysis pulse energies were  $\sim$ 4 mJ. For HCCl detection, 602.53 nm probe light ( $\sim$ 0.1–0.5 mJ pulse<sup>-1</sup>) was produced by a dye laser (Continuum ND-6000) pumped by the second harmonic of an Nd: YAG laser (Continuum Surelite II-10). The photolysis and probe beams were made collinear using a dichroic mirror and copropagated down a resistively heated Pyrex reaction cell. Fluorescence was detected at 90° from the laser beams using an R508 photomultiplier tube. Longpass filters were used to suppress detection of scattered laser light. The unamplified PMT signal was recorded by a boxcar integrator (Stanford Instruments Model 250) with a 500-ns delay and a 300-ns gate width and averaged on a personal computer. A digital delay generator (Stanford DG535) was used to vary the delay between excimer and dye laser pulses in order to produce a HCCl concentration vs. time profile. Control experiments were performed to verify that fluorescence signals at 602.53 nm originated from HCCl. Only upon photolysis of the precursor molecules were such signals observed.

For product molecule detection, infrared absorption spectroscopy was used as described in previous publications [9,10]. A tunable lead-salt diode laser provided the infrared probe radiation. The excimer and probe beams were made collinear with a dichroic mirror and copropagated through a 1.46-m absorption cell. The UV light was then removed with a second dichroic mirror, and the infrared light passed through a 0.25-m monochromator and was focused onto a 1-mm InSb detector (~1-µsec response). Transient infrared absorption signals were collected on a LeCroy 9310A digital oscilloscope and transferred to a computer for analvsis. The HITRAN molecular infrared database [11] was used as an aid in locating N<sub>2</sub>O absorption lines and calibrating absolute yields. HCNO and HNCO absorption lines were found with the aid of published infrared spectral data [12,13].

NO<sub>2</sub> (Matheson) was purified by vacuum distillation at 77 and 220 K. NO (Matheson) was purified by vacuum distillation at 180 K.  $CH_2CO$  (ketene) was synthesized by pyrolysis of acetic anhydride at 700°C and purified by vacuum distillation at 77 K.  $SF_6$  (Matheson) was purified by vacuum distillation at 77 K.  $CHClBr_2$ (Aldrich) was subjected to several freeze-pump-thaw cycles to remove dissolved air.

Typical reaction conditions in the LIF experiments were 0.1 Torr of CHClBr<sub>2</sub> and 0.005–0.06 Torr of NO or NO<sub>2</sub>. For the IR absorption experiments, typical conditions were 0.05 Torr of CHClBr<sub>2</sub>, 0–1.0 of Torr NO, and 1.0 Torr of SF<sub>6</sub> buffer gas. Based on an absorption coefficient of 0.097 cm<sup>-1</sup> Torr<sup>-1</sup> for CHClBr<sub>2</sub> at 193 nm, typical [HCCl]<sub>0</sub> number densities of  $\sim 3 \times 10^{13}$  cm<sup>-3</sup> were obtained (assuming a quantum yield of unity).

## RESULTS

#### **Total Rate Constants**

*HCCl* + *NO*. Laser-induced fluorescence signals at 602.53 nm with ~200 ns lifetimes were observed upon 193-nm photolysis of HCClBr<sub>2</sub>. Based on previous spectroscopic data [3], we can confidently assign these signals to the A(050)  $\leftarrow$  X(000) transition of the HCCl molecule. Figure 1 shows boxcar integrated signal amplitudes as a function of the delay time between excimer and dye laser pulses. As shown, the HCCl kinetic signals were found to be well approximated by single exponential decays over the range  $t = 10-120 \ \mu \text{sec}$ .

The decay rates were not significantly affected by the addition of He,  $N_2$ ,  $CF_4$ , or  $SF_6$  buffer gases. This



**Figure 1** Laser-induced fluorescence signals of HCCl as a function of excimer-dye delay time. Reaction conditions:  $P_{\text{HCClBr}_2} = 0.10$  Torr,  $P_{\text{NO}} =$  variable, T = 296 K.

observation suggests that vibrational relaxation effects are insignificant in these experiments. Either HCCl was produced vibrationally cold, or vibrational relaxation was accomplished within  $\sim 10 \,\mu$ sec even in the absence of buffer gas (if this were not true, we would expect to see slower rise times in Fig. 1). The magnitude of the LIF signals was lower in the presence of these buffer gases, presumably because of fluorescence quenching. As a result, most of the experiments were performed without any buffer gas.

Upon addition of nitric oxide to the reactant mixture, an increase in the HCCl decay rates was observed. In the presence of significant NO concentrations, pseudofirst-order conditions apply and a standard kinetic analysis shows that

$$[\text{HCCl}] = [\text{HCCl}]_0 \exp(-k't)$$
$$k' = k_1 [\text{NO}] + k_D$$

where k' is the observed pseudo-first-order decay rate constant,  $k_1$  is the desired bimolecular rate constant for the HCCl + NO reaction, and  $k_D$  represents the decay rate in the absence of added NO. Contributions to  $k_D$  include self-reaction, reaction with precursor molecules, and diffusion of detected species out of the probed volume. Although some of these processes are not strictly first order, the signals were found to be reasonably fit to pseudo-first-order kinetics even at low [NO]. Figure 2 shows k' as a function of [NO] at several different temperatures. The slope of these plots represents the bimolecular rate constant  $k_1$ .

Experiments on reaction (1) were conducted over the temperature range 298–572 K. Figure 3 shows an



Figure 2 Pseudo-first-order decay rates for HCCl as a function of NO pressure. Reaction conditions:  $P_{\text{HCClBr}_2} = 0.10$  Torr,  $P_{\text{NO}} =$  variable.



Figure 3 Arrhenius plot of the HCCl + NO rate constant.

Arrhenius plot of  $k_1$  over this range. The data are well fit to an Arrhenius expression:

$$k_1 = (2.225 \pm 0.05) \times 10^{-11}$$
  
  $\times \exp[(62.05 \pm 6.9)/T] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 

where the error bars represent one standard deviation. At 296 K, a value of  $k_1 = (2.75 \pm 0.2) \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> was obtained.

 $HCCl + NO_2$ . The addition of NO<sub>2</sub> to the reaction mixture caused a significant increase in HCCl pseudo-first-order decay rates, as shown in Fig. 4. Experiments



Figure 4 Pseudo-first-order decay rates for HCCl as a function of NO<sub>2</sub> pressure. Reaction conditions:  $P_{\text{HCClBr}_2} = 0.10$  Torr,  $P_{\text{NO}} =$  variable.



Figure 5 Arrhenius plot of the  $HCCl + NO_2$  rate constant.

over the temperature range 298–476 K were performed, as shown in Fig. 5. The data were well fit to an Arrhenius expression:

$$k_2 = (1.775 \pm 0.27) \times 10^{-9}$$
  
  $\times \exp[(-879.112 \pm 57.3)/T] \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 

At 296 K, a value of  $k_2 = (1.10 \pm 0.2) \times 10^{-10} \text{ cm}^3$ molecule<sup>-1</sup> s<sup>-1</sup> was obtained.

## **Product Branching Ratios**

The product branching ratio of reaction (1) was measured at 296 K using infrared absorption spectroscopy. HCNO, N<sub>2</sub>O, and CO<sub>2</sub> molecules were detected, as shown in the transient absorption signals of Fig. 6. Although the rise times for the various product molecules differ, this is probably because of vibrational relaxation kinetics rather than reaction kinetics. Since we probe only the ground vibrational state, the nascent vibrational distribution must be relaxed to a Boltzmann distribution in order for the molecular number densities to be reliably measured. SF<sub>6</sub> has previously been shown to be an efficient relaxer of vibrational excitation for N<sub>2</sub>O and CO<sub>2</sub> [14–16], and probably also relaxes HCNO as well. Under the experimental conditions of 1.0 Torr of SF<sub>6</sub>, this relaxation still takes about 50  $\mu$ sec for N<sub>2</sub>O and CO<sub>2</sub>, but is essentially complete on a timescale short compared to the slow decay, which is attributed to diffusion of molecules out of the probed volume.

The N<sub>2</sub>O and CO<sub>2</sub> products are believed to originate from a secondary reaction of NCO radicals formed in



**Figure 6** Transient infrared absorption signals for the products of the HCCl+NO and associated secondary reactions (see text). Lines probed: N<sub>2</sub>O (00<sup>0</sup>1)  $\leftarrow$  (00<sup>0</sup>0) R(3) at 2227.039 cm<sup>-1</sup>, CO<sub>2</sub> (00<sup>0</sup>1)  $\leftarrow$  (00<sup>0</sup>0) R(8) at 2355.890 cm<sup>-1</sup>, HCNO (0100<sup>0</sup>0<sup>0</sup>)  $\leftarrow$  (0000<sup>0</sup>0<sup>0</sup>) P(14) at 2184.608 cm<sup>-1</sup>. Reaction conditions:  $P_{\text{HCClBr}_2} = 0.05$  Torr,  $P_{\text{NO}} = 0.2$  Torr,  $P_{\text{SF}_6} = 1.0$  Torr.

reaction (1c) with nitric oxide:

$$NCO + NO \rightarrow N_2O + CO$$
 (3a)

$$NCO + NO \rightarrow CO_2 + N_2$$
 (3b)

This reaction has been studied in several laboratories [9,17–20]. It has a rate constant of  $(3.2–3.4) \times 10^{-11}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> at 296 K [17–19], with a moderate negative temperature dependence. The two product channels are formed in roughly equal yield [9,20], with  $\phi_{3a} = 0.44 \pm 0.07$  and  $\phi_{3b} = 0.56 \pm 0.07$ at 296 K. These branching ratios are virtually independent of temperature over the range 296–623 K [9].

The absolute concentrations of the detected products were determined as follows. For N<sub>2</sub>O and CO<sub>2</sub>, tabulated infrared absorption linestrengths are available [11], making absolute calibration straightforward, using formulae described in earlier publications [9,10]. These linestrengths have been checked by performing absorption measurements on static N<sub>2</sub>O and CO<sub>2</sub> gas, and found to be accurate to within 10% or better. For calibration of the transient signals, peak amplitues were used, and Doppler linewidths were assumed (pressure broadening is insignificant under the experimental conditions used). For fulminic acid (HCNO), no published linestrengths are available. HCNO, although not very stable, is not a transient species, so in principle absorption coefficients could be measured in a static cell. The synthesis of HCNO of known purity is rather difficult, however. An alternative approach was therefore used: Ketene (CH<sub>2</sub>CO) molecules were photolyzed at 193 nm. Although the dissociation of ketene at this wavelength is somewhat complicated, two products dominate [21,22]:

$$CH_2CO + h\nu(193 \text{ nm}) \rightarrow CH_2 + CO$$
 (4a)

$$CH_2CO + h\nu(193 \text{ nm}) \rightarrow HCCO + H$$
 (4b)

Channel (4a) is the major product, with  $\phi_{4a} = 0.81$ , and  $\phi_{4b} = 0.11$  [22]. Most of the methylene radicals are formed in the triplet ground state, and a small (<0.1) yield of CCO radicals was also observed [22]. In our calibration, typical conditions were 70 mTorr of CH<sub>2</sub>CO, 0.2–1.0 Torr of NO, and 1.0 Torr of SF<sub>6</sub> buffer gas. Under these conditions, [NO] > [CH<sub>2</sub>] and [NO] > [HCCO], so that essentially all of the CH<sub>2</sub> and HCCO radicals react with NO:

$$CH_2 + NO \rightarrow HCNO + H$$
 (5a)

$$CH_2 + NO \rightarrow HCN + OH$$
 (5b)

$$HCCO + NO \rightarrow HCNO + CO$$
 (6a)

$$HCCO + NO \rightarrow HCN + CO_2$$
 (6b)

The product branching ratios of these reactions have been previously studied. Several measurements of  $\phi_{6a}$ have been reported, with values of  $\phi_{6a} = 0.88 \pm 0.04$ [23] and  $0.64 \pm 0.12$  [24] at 296 K, and  $0.77 \pm 0.09$ [25] at 700 K. Only one group has reported a measurement of  $\phi_{5a}$ , with a value of 0.84 at 296 K [26]. What makes the calibration reliable is that fact the both of these reactions produce HCNO in similar yields. Thus every CH<sub>2</sub>CO molecule that is dissociated will produce approximately 0.8 HCNO molecules, essentially independent of uncertainties in the photolysis yields  $\phi_{4a}$  and  $\phi_{4b}$ . The number density of  $[CH_2]_0 + [HCCO]_0$  radicals produced in the ketene photolysis was obtained by measuring the 193-nm absorption coefficient of ketene sample (the values obtained varied substantially between different ketene samples because of different purity levels;  $CO_2$  impurity levels of ~30% are typical in our synthesized ketene samples) as well as the absolute excimer pulse energy incident upon the reaction cell, and assuming a total dissociation quantum yield of unity. The number density of HCNO was then determined by

$$[HCNO] = ([CH_2]_0 + [HCCO]_0) \times 0.84$$

where we used the value of  $\phi_{5a}$ , since channel (4a) is the dominant pathway for ketene dissociation. The peak–



**Figure 7** Product yields as a function of reagent NO pressure. Reaction conditions:  $P_{\text{HCCIBr}_2} = 0.05$  Torr,  $P_{\text{NO}} =$  variable,  $P_{\text{SF}_6} = 1.0$  Torr.

peak amplitude of the HCNO transient infrared signal was measured upon photolysis of a  $CH_2CO/NO/SF_6$  mixture. Comparison of this signal to the calculated [HCNO] provided the calibration factor which was then applied to the signals obtained from the title reaction.

Figure 7 shows the obtained number densities of N<sub>2</sub>O, CO<sub>2</sub>, and HCNO as a function of reagent NO pressure. Several conclusions can be obtained from this result. The product yields quickly level off at  $P_{\rm NO} > 0.2$  Torr, indicating that at these NO pressures, essentially every HCCl radical produced in the dissociation reacts with NO. The ratio of [HCNO] in the high pressure limit of Fig. 7 to the initially produced [HCCl]<sub>0</sub> concentration may therefore be taken as an accurate estimate of the branching ratio  $\phi_{1a}$ . Furthermore, the fact that the observed N2O and CO2 yields are roughly equivalent provides evidence that these products do indeed originate from secondary reactions of NCO radicals, reaction (3), which produces  $N_2O$  and  $CO_2$  in similar yields. The product branching ratio for NCO formation,  $\phi_{1c}$ , can therefore be determined by

$$\phi_{1c} = [N_2O]/(0.44 \times [HCCl]_0)$$

where we have assumed that every NCO radical created in reaction (1) reacts with NO. Using the above techniques, we obtain the following branching ratios for reaction (1) at 296 K:  $\phi_{1a} = 0.68 \pm 0.06$  and  $\phi_{1c} = 0.24 \pm 0.04$ , where the error bars represent one standard deviation.

Several possible product channels were not detected in this experiment. Attempts to detect HNCO transient signals were unsuccessful. We estimate  $\phi_{1b} < 0.1$ . No

## DISCUSSION

Our value for the HCCl + NO rate constant at 296 K is somewhat higher than that of the one previous study of this reaction, which reported  $k_1 = (1.5 \pm 0.5) \times$  $10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$  [5]. We do not have any explanation for the discrepancy, except to note that HCCl fluorescence signals are quite weak and careful filtering is required to eliminate background signals from scattered laser light. Our work represents the first reported value of  $k_2$  as well as the branching ratios of reaction (1). Although neither the NCO nor HCl product from channel (1c) was directly detected, we are quite confident about the existence of this channel because the NCO + NO reaction is the only reasonable source of the detected N<sub>2</sub>O product molecules in this system. In principle both of these products could be detected by IR absorption, but their infrared linestrengths are substantially smaller than those of N<sub>2</sub>O, so that our indirect method is the more sensitive approach.

In the product channel measurements, we assumed that the CHClBr<sub>2</sub> photolysis produced HCCl radicals with a quantum yield of unity. No previous experimental evidence for this assumption exists, however our results strongly suggest that this assumption is approximately correct. If the quantum yield were much less than one, then the sum of our observed branching ratios would also be less than one. Our value of  $\phi_{1a} + \phi_{1c} = 0.92$  is close to unity, within experimental uncertainties, however.

Formation of the major channel (1a) can proceed by a straightforward mechanism, involving formation of an HC(Cl)NO intermediate followed by C–Cl bond cleavage. A possible mechanism for NCO formation in channel (1c) is formation of a three-member CNO ring, followed by H atom migration to the Cl atom, ring opening, and subsequent C–Cl fission. Another less likely possibility, which we cannot directly probe, would be formation of the high energy isomer CNO rather then NCO.

## CONCLUSIONS

The reactions of HCCl with NO and  $NO_2$  are fast with only a very slight temperature dependence. Analysis of products of the HCCl + NO reaction indicates that HCNO + Cl is the major channel, with a smaller contribution from NCO + HCl.

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