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# Collisional excitation of $CO_2(00^00)$ vibrationless state by the highly translationally excited HCN produced from the photodissociation of *s*-triazine

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## Abstract

The collisional excitation of $CO_2(00^00)$ state by quenching of highly translationally excited HCN has been studied with high-resolution diode laser absorption spectroscopy. The translationally hot HCN is produced from the photodissociation of *s*-triazine (1,3,5-triazine) at 266 nm. The average translational energy of HCN is measured to be 18 ± 1 kcal/mol, which corresponds to 84% of available energy for the HCN fragment. The fraction of available energy partitioned into the rotational excitation is 15%. A little excitation in the HCN bending vibration is observed. The nascent rotational excitation in the $00^00$ levels of $CO_2$, due to collisions with the translationally hot HCN (from *s*-triazine), is accompanied by a substantial enhancement in the translational energy. The excitation in the translational recoil velocities appears to increase with increasing $J$ in $00^00$ vibrational state. © 1998 Elsevier Science B.V. All rights reserved.

## 1. Introduction

Despite numerous interest for collisional relaxation phenomena, the detailed mechanism for the collisional energy transfer between the translationally hot molecule and a bath gas collision partner has not yet been established at the quantum-state resolved level. Recently, high-resolution (infrared) IR diode laser devices have been used to probe the vibrational, rotational and translational energy of bath molecules, thereby providing details of the energy transfer process that have not in general been available using other experimental methods. In this work, the quantum resolved details in the collisional relaxation of translationally hot HCN by a $CO_2$ bath is investigated using the IR diode laser probe technique.

It is well established that *s*-triazine (1,3,5-triazine) yields three HCN fragments following the absorption of a photon. In the past years, the photodissociation of *s*-triazine has been of great interest because of the high symmetry of the dissociation process, each excited *s*-triazine molecule yielding three HCN molecules. Ondrey and Bersohn measured the translational energies of the HCN fragments produced at the excitation wavelength of 248 and 193 nm by TOF technique [1]. They suggested that the initial 3-fold symmetry would be retained during

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dissociation and that dissociation must take place from the ground state of the parent molecule, and is therefore likely to generate nearly equal speeds in all fragments. They measured that the HCN molecules have an average kinetic energy of 10 kcal/mol (41% of the available energy) at 248 nm but only 2 kcal/mol (11% of the available energy) at 193 nm. Goates et al. observed the vibrationally excited HCN molecules produced from the photodissociation of *s*-triazine at 193 nm by IR fluorescence spectroscopy [2]. Recently, Huber and his coworkers reported the average translational energy of HCN produced from the photodissociation of *s*-triazine at several ultraviolet (UV) wavelengths by using the molecular beam photofragment translation spectroscopy, and argued that the dissociation mechanism is a two-step concerted process rather than simultaneous one-step process [3]. They measured the translational energies of HCN molecules to be about 55% and 70% of available energy at 193 nm and other wavelengths (248, 275, 285 and 295 nm), respectively, which are quite different from the result reported by Ondry and Bersohn. Therefore, it is necessary to determine the translational-state distribution of HCN before undertaking the collisional energy transfer involving HCN molecule. A high-resolution diode laser was employed to probe the state-specific energy deposition in the HCN produced from the photodissociation of *s*-triazine.

The basic experimental scheme can be illustrated by the following equations:

$$s-\text{triazine}+h\nu(266\,\text{nm})\rightarrow 3\text{HCN}(mn^lp,J,V)\qquad(\text{HCN production})$$

$$\text{HCN}(mn^lp,J,V)+h\nu(\sim 3.1\,\mu\text{m})\rightarrow \text{HCN}(mn^lp+1,J\pm 1,V)\qquad(\text{Diode laser probe})\,,$$

where $m$, $n$ and $p$ are the quantum numbers for the symmetric stretching $(\nu_1)$, bending $(\nu_2)$ and asymmetric stretching $(\nu_3)$ vibrational modes. $J$ and $l$ denote, respectively, the rotational and vibrational angular momentum quantum numbers and $V$ denotes the translational velocity along the direction of the diode beam. The nascent translational-, rotational- and vibrational-state distributions of HCN were probed in the P branch of the strongly allowed antisymmetric stretching band at ~ 3.1 μm. The experimental results as described in the following sections show that the HCN molecule carries high translational energy such as $18\pm 1$ kcal/mol.

High-resolution single-collision study on the energy transfer between the translationally excited HCN molecule produced from the photodissociation of *s*-triazine and $CO_2$ bath molecule were performed. The IR diode laser probe technique is also used to measure the rotational and translational excitation of vibrationally ground $CO_2$ resulting from the collisions with the translationally hot HCN. It provides the information in exquisite detail about the energy transfer process from translationally hot triatomic molecule to the quantum states of $CO_2$ bath acceptor molecules. The basic experimental approach is described by the following equations:

$$s-\text{triazine}+h\nu(266\,\text{nm})\rightarrow 3\text{HCN}\qquad(\text{HCN production})\,,$$

$$\text{HCN}+\text{CO}_2\rightarrow \text{HCN}+\text{CO}_2(mn^lp,J,V)\qquad(\text{Collisional quenching})\,,$$

$$\text{CO}_2(mn^lp,J,V)+h\nu(\sim 4.3\,\mu\text{m})\rightarrow \text{CO}_2(mn^lp+1,J\pm 1,V)\qquad(\text{Diode laser probe})\,.$$

The nascent rotational populations and translational recoils of $CO_2$ within the ground vibrational manifold are probed in the P branch of the strongly allowed antisymmetric stretching band at 4.3 μm.

## 2. Experimental

The diode laser absorption technique has been described in detail previously and only a brief description is given here [4–6]. The photolysis laser is a Continuum Nd:YAG 266 nm laser. For measuring the nascent-state distributions of HCN produced by photodissociation, a 3.1 μm cw diode laser (Mütek) is propagated collinearly with the UV laser beam through a 2.7 m Pyrex cell containing less than 8 mTorr. All measurements were made with Nd:YAG laser repetition rates of 0.1 ~ 0.15 Hz in order to ensure the pumping of residual gas. For the collision experiment, a 4.3 μm cw diode laser (Mütek) is propagated co-linearly with the UV laser beam through a 2.0 m Pyrex cell containing approximately 13 mTorr of a flowing 1:4 gas mixture of *s*-triazine and $CO_2$. The IR light intensity transmitted through the cell is measured using a liquid nitrogen-cooled InSb photodetector which, together with its amplifier, has a rise time of approximately 450 ns. In order to insure that the detected IR light from a single laser mode, the transmitted IR is passed through a monochromator before being focused onto the photodetector. The absorption signals are recorded and averaged over 1000 cycles of the modulated diode laser by a LeCroy 9354A digital oscilloscope.

Transient IR absorption signals are collected with the diode laser locked to the center of the relevant absorption line. The signal from this detector is used as the reference for an SR510 lock-in amplifier (Stanford Research Systems). This arrangement allows the diode laser frequency to be locked to any absorption line of interest. The transient absorption signal is input into two channels on the digital storage oscilloscope, one ac-coupled and the other dc-coupled. The ac-coupled channel records $\Delta I$, the change in IR absorption while the dc-coupled channel represents $I + \Delta I$, the absolute intensity of the transient of IR signal. For each excimer shot, the ac-coupled signal is divided by the dc-coupled signal to yield $\Delta I/(I + \Delta I)$, which can be algebraically rearranged to give $(\Delta I/I)$, the desired quantity on a shot-to-shot basis without the use of a pair of matched detectors. Transient signals are typically averaged over ~ 70 excimer shots fired. Additionally, a reference line technique is used for all population measurements in order to account for change in the signal intensity due to long-term drifts in the system.

Active locking of the diode laser frequency to a HCN or $CO_2$ absorption line is accomplished using a separate reference cell. A fraction (~ 10%) of the diode beam is sent through a reference cell and a monochromator and detected by an additional InSb detector. The IR absorption signal from the reference detector is input to a lock-in amplifier, the output of which is used as an error signal sent to the diode laser controller, thus keeping the diode laser frequency locked to the absorption transition.

For the line-width measurements, the diode laser frequency was locked to an IR fringe of a Laser Photonics Confocal Etalon (Model SP 5945) using a 1 kHz modulation frequency. The modulation amplitude was roughly the width of a fringe, 0.002 $cm^{-1}$, and precise diode laser frequency control was accomplished by computer-controlled rotation of a scanner plate internal to the etalon. Transient absorption signals were obtained while the etalon fringe was over the absorption line of interest. The excimer laser was fired at the center of the modulation cycle in order to sample only a single diode laser frequency for a given etalon fringe position.

*s*-Triazine (Aldrich, 97%) was purified by several freeze (77 K)–pump–thaw cycles. Research grade $CO_2$ (Matheson, 99.995%) was used without further purification.

## 3. Results and discussion

### *3.1. Translational, rotational and vibrational energy distribution of HCN produced from the photodissociation of s-triazine*

The Doppler profile of the $HCN(00^00, J = 23) \rightarrow HCN\ (00^01, J = 22)$ absorption line at 3238.20 $cm^{-1}$ is shown in Fig. 1a. The Doppler profiles were measured at 450 ns after the excimer laser pulse. The pressure of *s*-triazine was 4 mTorr and the repetition rate of photolysis laser was 0.1 Hz. The full width at half maximum (FWHM) averaged over this line and other rotational lines such as $HCN(00^00, J = 22) \rightarrow HCN(00^01, J = 21)$ and $HCN(00^00, J = 20) \rightarrow HCN(00^01, J = 19)$ is $0.040 \pm 0.002$ $cm^{-1}$. However, when 8.5 mTorr of *s*-triazine is used, the top of Doppler profile becomes less flat and its FWHM is reduced by a few percent, indicating the Doppler profile measured even at 4 mTorr may not reveal the nascent velocity distribution of HCN. The Doppler profiles of $HCN(01^10, J = 14) \rightarrow HCN(01^11, J = 13)$ and $HCN(01^10, J = 17) \rightarrow HCN(01^11, J = 16)$ absorption lines have been measured for 4 mTorr and 8.5 mTorr of *s*-triazine, showing the same FWHM as $0.040 \pm 0.002$ $cm^{-1}$. The Doppler profile of $HCN(01^10, J = 14) \rightarrow HCN(01^11, J = 13)$ at 8.5 mTorr is shown

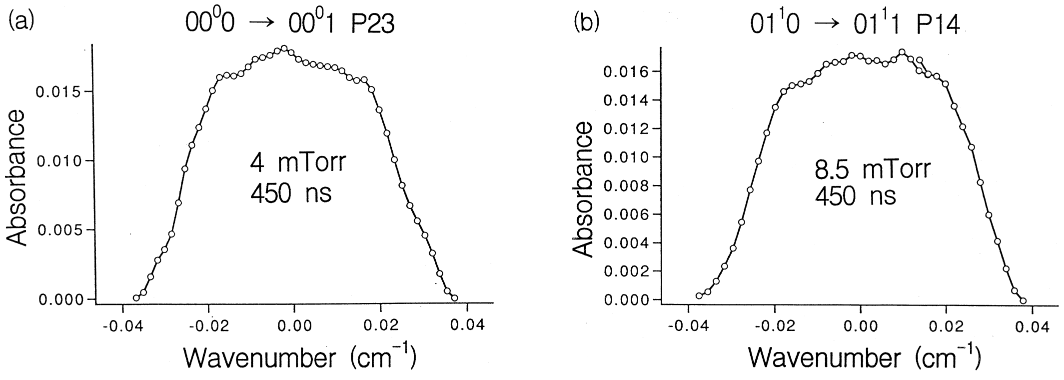

Fig. 1. (a) Nascent Doppler profile line shapes of the HCN($00^00$, $J=23$) → HCN($00^01$, $J=22$) absorption line produced by photodissociation of 4 mTorr *s*-triazine. The FWHM is 0.04 $\mathrm{cm}^{-1}$. (b) The Doppler profile of the HCN($01^10$, $J=14$) → HCN($01^11$, $J=13$) absorption line produced by photodissociation of 8.5 mTorr *s*-triazine. The FWHM is 0.04 $\mathrm{cm}^{-1}$. The Doppler profiles (a) and (b) were measured at 450 ns after the excimer laser pulse and the repetition of Nd:YAG 266 nm laser was 0.1 Hz.

in Fig. 1b, which is similar to Fig. 1a. The pressure effect on the Doppler profiles of $00^00$ rotational lines is due to the thermal HCN quenched from other highly excited ro-vibrational states. We took the averaged FWHM for several HCN($00^00$) → HCN($00^01$) and HCN($01^10$) → HCN($01^11$) transition lines as $0.040 \pm 0.002\ \mathrm{cm}^{-1}$.

If the velocity distribution is isotropic, which cannot be checked under our collinear pump and probe beams alignment, the velocity distribution can be obtained from the first derivative of the Doppler profile. The average translational energy of HCN is calculated to be 18 ± 1 kcal/mol, which is consistent with 17 kcal/mol reported by Huber and coworkers for the 248 nm photodissociation of *s*-triazine. The reaction enthalpy for the dissociation is known as 43.0 kcal/mol, so the fraction of available energy partitioning into translational state is 84%.

Typical time-resolved signal observed while monitoring the HCN($00^00$, $J=20$) → HCN($00^01$, $J=19$) transition line at 3248.48 $\mathrm{cm}^{-1}$ is shown in Fig. 2a. The IR diode laser light absorbed in the $v \rightarrow v+1$ transition is proportional to the population difference between $v$ and $v+1$ levels:

$$N(v,J) - N(v+1,J \pm 1) \propto (\Delta I/I_o)/\left[X_J R^2 \nu\right], \tag{1}$$

where $\Delta I$ is the change in the amount of IR light transmitted following the reaction, $I_0$ is the total IR intensity at frequency $\nu$, $X_J$ is the Hönl–London factor given by $(J+1)/(2J+1)$ for R branch lines and $J/(2J+1)$

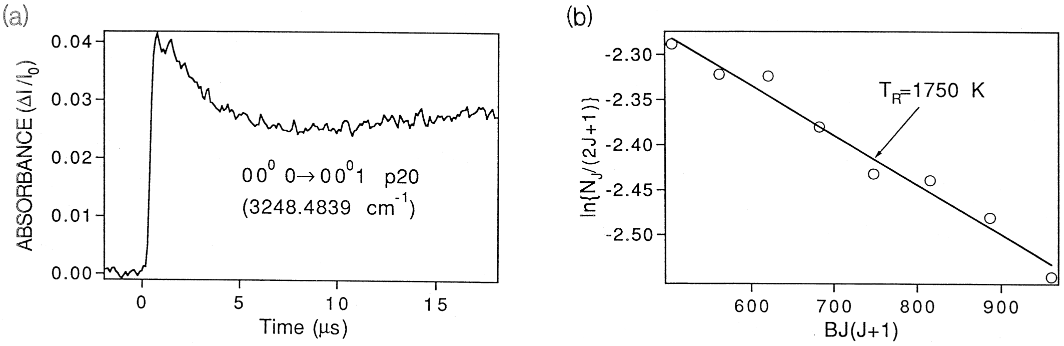

Fig. 2. (a) Time-resolved absorption signals observed while monitoring the HCN($00^00$, $J=20$) → HCN($00^01$, $J=19$) transition line at 3248.48 $\mathrm{cm}^{-1}$. The pressure of *s*-triazine is 4 mTorr and the repetition of Nd:YAG laser was 0.1 Hz. (b) Boltzmann plot of the nascent rotational distribution of HCN($00^00$) produced by the photodissociation of *s*-triazine. The line is the best fit to a rotational temperature of 1750 K. The $N_J$ is the experimentally determined number of molecule produced in a given rotational state of HCN.

for P branch lines and $R$ is the transition matrix element. In the present experiment, the upper-state population has been determined to be negligible compared to the lower-state populations. Thus the observed transient absorption signals reflect the temporal behavior of the population in the lower ro-vibrational level only. The nascent population of ro-vibrational states was obtained by measuring the absorption signal amplitude at 500 ns after the excimer laser pulse. In order to confirm that the observed transient absorption signals come from single photon absorption of *s*-triazine, the absorption signals have been measured as a function of laser intensity, showing a good linearity. The rotational Boltzmann plot of the nascent rotational-state distribution of HCN($00^00$) is shown in Fig. 2b. The best fit to a Boltzmann distribution gives a temperature of $T_R = 1750$ K. The average of several experimental runs provides $T_R = 1750 \pm 100$ K for the $00^00$ state and $T_R = 1350 \pm 100$ K for the $01^10$ state. The rotational-state distribution has been measured for $J = 17$–$25$ for $00^00$ state, and $J = 11$–$19$ for $01^10$ state. Since the translational energy distribution of $00^00$ and $01^10$ states are about same, the rotational temperature can be expected to be similar, which is consistent with the results. The rotational temperature of HCN is ~ 5 times of room temperature and the average rotational energy is $3.2 \pm 0.2$ kcal/mol. Thus the fraction of available energy partitioned into the rotational excitation is 15%.

Since the translational- and rotational-state distributions for the $00^00$ and $01^10$ states of HCN were measured, the relative populations of these two vibrational levels were determined by measuring relative absorption amplitudes for some rotational levels in the $00^00$ and $01^10$ states. The population ratio of $01^10$ to $00^00$ state is 0.4. The population in other vibrational states was found to be negligible. Therefore, about 70% of HCN fragments is in the vibrational ground state, and an average vibrational energy is estimated to be $0.5 \pm 0.1$ kcal/mol above the HCN zero point level, which is close to the residual energy calculated by subtracting the average translational energy and rotational energy from the available energy of HCN. Table 1 lists the average translational, rotational and vibrational energies of the HCN molecules produced by the photodissociation of *s*-triazine at 266 nm.

The UV absorption spectrum of *s*-triazine in the region of 238–326 nm shows two overlapping $n \rightarrow \pi^*$ transitions; a very weak one which is due to the forbidden doubly degenerated $^1A_1 \rightarrow {}^1E''$ and a much stronger one which is due to the symmetry allowed $^1A_1 \rightarrow {}^1A_2''$ [7]. The transition dipole moment for the transition $^1A_1 \rightarrow {}^1A_2''$ is perpendicular to the molecular plane of *s*-triazine. It is known that *s*-triazine is simply decomposed to three HCN molecules. There are two likely mechanisms for the photodissociation of *s*-triazine. The one is a symmetric simultaneous single process and the other one is a sequential process. In the case of single step dissociation, three HCN fragments have same kinetic energy in the center-of-mass frame of *s*-triazine molecule, and in the case of sequential reaction two different translational energies are expected.

Recently, Pai et al. calculated the stable points and the transition states along the reaction path for a concerted triple and a stepwise decomposition mechanisms of *s*-triazine by using non-local density functional methods (NDFT) and ab initio methods [8,9]. All methods predict that the low-energy pathway to decomposition is a concerted triple dissociation and that a weakly bound cyclic $(HCN)_3$ clusters exists on the reaction path. Osamura et al. also concluded that the triple dissociation of *s*-triazine occurs on the ground-state potential surface and is a one-step concerted reaction from the ab initio calculations [10]. All these calculations for the geometry and nuclear motion of the transition state show that the bending mode of HCN should be excited in HCN molecules after the dissociation, which is consistent with our result. Unfortunately, the translational

Table 1
Average energy partitioning of HCN

| $h\nu$ | $E_{AVAL}$ | $3\langle E_T \rangle$ | $3\langle E_R \rangle$ | $3\langle E_V \rangle$ |
|---|---|---|---|---|
| 107.7 | 64.5 | 54 (84%)[a] | 9.7 (15%) | 1.5 (2%) |

$E_{AVAL} = h\nu$-dissociation energy, $\langle E_T \rangle$, $\langle E_R \rangle$ and $\langle E_V \rangle$ are the average total translational, rotational and vibrational energy, respectively. All energies are in unit of kcal/mol.

[a] The percentage of available energy.

energy distribution derived from the Doppler profile of ro-vibrational absorption line cannot give a definite evidence for the concerted dissociation mechanism. Thus a sequential process could occur on similar time scale, as suggested by Huber and his coworkers [3].

### 3.2. Energy transfer from translationally hot HCN to $CO_2$

Transient populations of $CO_2$ molecules in $J = 62$, 72, 74, 78, 80 and 82 states of the ground vibrationless level were monitored via IR diode laser absorption. A typical transient signal is shown in Fig. 3a, where the absorption on the $CO_2(00^00, J = 74) \rightarrow CO_2(00^01, J = 73)$ line at 2274.99 $cm^{-1}$ is plotted against the time relative to the excimer laser pulse. The early, linear rise in the signal represents predominantly single collision excitation of $CO_2$ to $J = 74$ by translationally hot HCN. The total pressure of the 1/4 *s*-triazine/$CO_2$ mixture is adjusted to be 13 mTorr such that the mean time between ambient gas collisions is 2.3 μs, which is much slower than the detector response time. The fast rise component of the signals is due to nascent rotational excitation of $CO_2$ by fast HCN. The nascent rotational distribution is shown in Fig. 3b. As described below, the transient linewidths for $J = 62$, 74 and 80 were also measured. Because the linewidth increases as a function of rotational level $J$, one must integrate over the line shape in order to obtain rotational-state populations. All line shapes fit exactly to the Gaussian functions, the signal at the line center was therefore corrected by the linewidth. The nascent populations of $J = 72$, 78 and 82 rotational states are corrected by the interpolated linewidth from the measured one of $J = 62$, 74 and 80 on the assumption that the FWHM increases linearly with increasing $J$. The resulting rotational-state distributions fit a Boltzmann distribution with the temperature of $1300 \pm 130$ K, based on data for the states $J = 62$–82.

The recoil velocities onto the probe beam axis were determined from the measurements of the Doppler broadened line shape. All of the measured line shapes fit well to Gaussian forms, and the FWHM of Doppler profile for the absorption transitions $J = 62$, 74 and 80 are $0.011 \pm 0.005$, $0.0125 \pm 0.005$ and $0.0140 \pm 0.005$, respectively, as shown in the inset of Fig. 3b. Note that these linewidths are measured at $t = 700$ ns after the excimer laser pulse. The linewidth of a transition probing $CO_2$ molecules with a room temperature velocity distribution is 0.00425 $cm^{-1}$. Clearly $CO_2$ molecules which are rotationally excited in high $J$ states by the collisions with fast HCN possess a large amount of translational energy and the translational recoil velocity increases substantially as $J$ increases from 62 to 82.

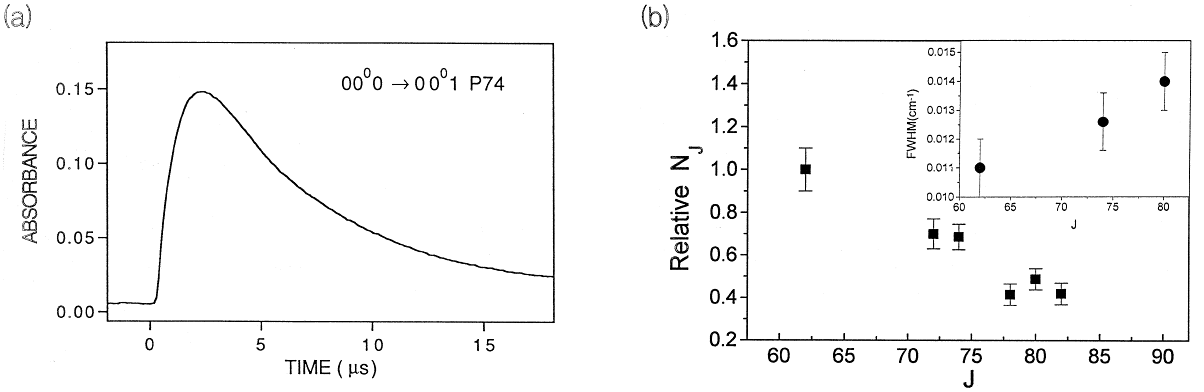

Fig. 3. (a) The transient signal observed while monitoring the $CO_2(00^00, J = 74) \rightarrow CO_2(00^01, J = 73)$ transition line at 2274.99 $cm^{-1}$. The total pressure of the 1/4 *s*-triazine/$CO_2$ mixture is 13 mTorr. (b) Rotational population distribution of $CO_2$ in high $J$ levels of the $00^00$ state produced by translationally excited HCN. The inset is the FWHM of the $CO_2$ $00^0000^01$ transition as a function of rotational level $J$. The line widths are measured at $t = 700$ s after the laser pulse.

A simple billiard ball model predicts a translational energy transfer of $\Delta E = \left[2 M_{\mathrm{HCN}} M_{\mathrm{CO}_2} / \left(M_{\mathrm{HCN}} + M_{\mathrm{CO}_2}\right)^2\right] E_0$, where $M_{\mathrm{HCN}}$ and $M_{\mathrm{CO}_2}$ are the HCN and $CO_2$ mass and $E_0$ is the translational energy of hot HCN [11]. For a hard-sphere collision between HCN and $CO_2$, 47% of the HCN translational energy may be transferred. This equation roughly predicts only the magnitude of the translational recoil, thus a detailed trajectory calculation needs to explain the linewidth dependence of the $00^00$ states. A similar rotational dependence was observed in the transient linewidth measurement for the collisional excitation of $CO_2$ by hot atoms [11]. The breathing ellipsoid model was used to model the collisional energy transfer between hot hydrogen atom and $CO_2$ [12]. This model can be examined for the collision between hot HCN and $CO_2$ as a future work.

The collisional energy transfer from the vibrationally excited pyrazine to bath $CO_2$ was studied by Flynn and his coworkers [4–6]. Chesko et al. reported that pyrazine can be dissociated at a significant yield of HCN which can recoil and produce the excited $CO_2$.by the collisions [13]. Flynn and coworkers carried out the experiment to probe HCN evolution and found that the extent of dissociation is small at 1 μs delay time used in their experiments and thus the energy transfer is not affected significantly [14]. The translational energy of HCN produced from the *s*-triazine measured in this work is about same as that of HCN produced from the photodissociation of the pyrazine at 248 nm measured by Chesko et al. However, the transient absorption of rotationally excited $CO_2$ produced by translationally hot HCN in this study (Fig. 3a) show the faster rise rate than that of the $CO_2$ excited by vibrationally excited pyrazine in the work of Flynn and his coworkers. Furthermore, the translation recoils of $CO_2$ produced by translationally hot HCN are different from those of $CO_2$ in the Flynn and his coworkers' work. Therefore, we also conclude that in the case of pyrazine, the collisional $CO_2$ excitation by HCN is insignificant.

## 4. Conclusions

The collisional quenching of translationally excited HCN by $CO_2$ were studied with high-resolution diode laser absorption spectroscopy. It is first time to study the collisional energy transfer between the translationally excited triatomic molecule and bath molecule at a quantum-state resolved level. The translationally hot HCN are produced from Nd:YAG 266 nm photodissociation of *s*-triazine. The translational- and rotational-state distributions in $00^00$ and $01^10$ vibrational states of HCN were probed at 450 ns following the excitation by laser pulse. On the assumption of isotropic velocity distribution, the average translational energy HCN is estimated to be $18 \pm 1$ kcal/mol, which is 84% of available energy of HCN fragment. The average rotational energy of HCN is $3.2 \pm 0.2$ kcal/mol, thus the fraction of available energy partitioned into the rotational excitation is 15%. A little excitation in the bending vibration is observed. The nascent rotational excitations in the $00^00$ vibrational levels of $CO_2$ produced by translationally hot HCN are accompanied by a substantial enhancement in the $CO_2$ translational energy, and the translationally recoil velocity increases substantially with rotational level. A detailed trajectory calculation needs to explain the experimental results.

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