# Infrared Spectra and Isomerization of CHNO Species in Rare Gas Matrices

# V. E. BONDYBEY AND J. H. ENGLISH

Bell Laboratories, Murray Hill, New Jersey 07974

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# C. WELDON MATHEWS AND R. J. CONTOLINI

Department of Chemistry, The Ohio State University, Columbus, Ohio 43210

Infrared and uv absorption spectra of the CHNO isomers in rare gas matrices and their photolysis products by ultraviolet light were studied. The most efficient processes occurring in the matrix involve isomerization between the CHNO species. The NCO free radical is the only fragment appearing in the ir spectrum. The diatomic fragments CN, NH, and OH are also observable in the uv spectrum of photolyzed samples.

#### INTRODUCTION

The present research was started with the intent of generating and spectrally characterizing the CNO radical. In a recent manuscript (1), we have indeed reported the electronic absorption spectrum of this radical in solid Ne. However, unlike its NCO isomer (2-4), the excited electronic state of CNO exhibits no observable fluorescence in solid neon, and therefore only upper-state vibrational frequencies could be obtained. We therefore attempted to obtain information about the CNO ground state by direct infrared observation. Unfortunately, the uv radiation which produces CNO by photolysis of fulminic acid, HCNO, also causes secondary CNO isomerization into NCO, and concentrations of CNO sufficient for ir detection could not be stabilized. In the course of this work, however, rather extensive information about the ir spectra of the CHNO isomers and their rearrangements in the rare gas solids was obtained. The CHNO molecules, containing one atom each of the four principal elements of organic matter, are of considerable interest and have been the subject of extensive experimental and theoretical studies (5-8). We therefore decided to report our results in this manuscript.

While numerous topologically different CHNO structures can be written, only relatively few of these appear reasonable in terms of our present understanding of chemical bonding. This is confirmed by theoretical ab initio calculations. At the highest computational level used, Poppinger *et al.* (8) find only seven distinct potential minima. Only four of the minima appear to be sufficiently deep and well defined to suggest their independent existence as stable isomers. Experimentally two of these, fulminic acid and isocyanic acid and their salts, were known since

the early days of chemistry (9, 10), although their structures were elucidated only relatively recently (11, 12). The most extensive information about their geometry comes from spectroscopic studies, both in the infrared and in the microwave region. The experimental evidence (13-18) shows that HNCO is bent with  $\neq$  HNC  $\sim 128^{\circ}$ , while fulminic acid, HCNO, is best described as quasilinear (19-25). The HCN bending potential function exhibits a small barrier to linearity which is, however, well below the lowest vibrational level (26).

Using careful matrix isolation studies, Jacox and Milligan have presented evidence for the stabilization of cyanic acid, HOCN, and its deuterated counterpart (27). Although ab initio calculations suggest that also isofulminic acid, HONC, should be sufficiently stable to permit its isolation, to date there appears to be no experimental evidence for its existence.

#### EXPERIMENTAL DETAILS

The fulminic acid was prepared by pyrolysis of 4-phenyl isoxazolinedione monoxime (28) as recently described by Wentrup and co-workers (29). Isocyanic acid was prepared by thermal decomposition of its cyclic trimer, cyanuric acid (30). For preparation of DNCO, the cyanuric acid was first recrystallized several times from  $D_2O$ . DCNO was prepared from HCNO by repeated exchanges with  $D_2O$  in the vapor phase. All compounds were purified by vacuum distillation and stored at liquid nitrogen temperature.

Dilute solutions of the above compounds in neon or argon (1:500-1:2000) were prepared by standard gas-volumetric techniques. The solutions were deposited on a CsI window held at 4 K. Photolysis of the samples was accomplished using an Oriel 50-W high pressure xenon lamp or by atomic resonance lamps powered by a microwave discharge (75 W).

Infrared spectra of the deposits before and after photolysis were obtained using a Nicolet-MX-1 Fourier transform infrared spectrometer.

# **RESULTS AND DISCUSSION**

# (a) Spectrum of Isocyanic Acid

The infrared spectrum of HNCO has been studied very extensively (13-18), yet some uncertainties remain regarding its vibrational assignment. The main controversies involved the three low-frequency modes which can be approximately described as HNC angle bending, and in- and out-of-plane bending of the NCO group. It is therefore perhaps of interest to compare our Ne matrix spectra with the recent gas phase spectroscopic studies (18, 31).

The matrix spectrum of HNCO is shown in Fig. 1 and the results are compared with the most recent gas phase data in Table I. The three stretching frequencies are readily identified and are in satisfactory agreement with the gas phase values.  $\nu_2$ , the asymmetric stretch of the NCO entity, is the strongest band in the spectrum at 2268 cm<sup>-1</sup>, while the symmetric stretch  $\nu_3$  is very weak and appears at 1320 cm<sup>-1</sup>. Both of these values are close to the corresponding modes of CO<sub>2</sub>. Interestingly, the  $\nu_3$  band of DNCO, reported at 1310 cm<sup>-1</sup> in the gas phase by Ashby and Werner (31), was not observed in the matrix and must be considerably weaker than the corresponding mode of HNCO. This may be due to the fact that the DN group is closer in mass to that of O atom, and thus in the deuteride,  $v_3$  will be to a better approximation a "symmetric" stretching mode than in the hydride.

The bending frequencies of the HNCO molecule are in good accord with the gas phase spectrum. Their relative intensities also provide some interesting information. While in the gas phase  $v_6$  appears with intensity comparable to the in-plane bending modes (12) and is in fact stronger than  $v_5$ , in the matrix it is weaker by more than an order of magnitude. In the gas phase it was noted that the intensity of the subbands increases with increasing value of K. No bands involving the K = 0 level were observed (18) and are apparently very weak. The low intensity of  $v_6$  in the matrix where, at 4 K, only the K = 0 level will be thermally accessible is therefore consistent with these gas phase observations.

By far the most serious discrepancy between the gas phase and the matrix involves  $\nu_4$  in DNCO. Ashby and Werner (31) report this vibrational mode (essentially NCO in-plane bend) at 766.8 cm<sup>-1</sup>, while in the matrix a strong band at 722.4 cm<sup>-1</sup> is observed. While one might attribute this to a matrix shift, this appears quite unlikely, since all the other vibrational modes of both HNCO and DNCO appear in the matrix within 1-5 cm<sup>-1</sup> of their gas phase positions. Furthermore, the  $\nu_4$  mode is observed also in Ar matrix at very nearly the same position as in Ne. It appears that a reexamination of the gas phase data would be worthwhile.

# (b) Infrared Spectra of Fulminic Acid

The spectra of HCNO were previously extensively studied and are well understood. The Ne matrix spectrum is shown in Fig. 1a and the results are summarized in Table II. The three stretching vibrations  $\nu_1 - \nu_3$  appear at 3336, 2196, and 1254 cm<sup>-1</sup>, respectively, in each case within a few cm<sup>-1</sup> of their gas phase position. The

			HNCO		DNCO		
		Gas*	Ne	Ar	Gasð	Ne	Ar
¥6	δNCO <sub>1a2</sub>	660	668.4		602.9		
¥ 5	$\delta NCO_{1}a_{1}$	577.3	575.8	572.9	460.	460.1	458.1
¥ 4	δHNC	77 <b>6</b> .6	773.5	769.7	766.8	722.4	721.4
v 3	₽5NCO	1327.	1320.4		1310.		
V 2	NCOو	2274.	2268.4	2259.8	2235.	2240.4	2231.8
<b>v</b> 1	⊮HN(DN)	3531.	3537.7		2634.9	2635.9	

## TABLE I

Vibrational Frequencies of HNCO in Solid Ar and Ne and Their Comparison with the Gas Phase

\* Gas phase frequencies taken from Refs. (17, 18).

<sup>b</sup> From Ref. (31).





same region showing the effects of 10-min photolysis of by a 50-W Xe arc lamp. Vibrational bands of cyanic acid, HOCN, are labeled. The unlabeled positive Fig. 1. (a) Sections of the matrix spectrum of HCNO in Ne matrix. The strongest HCNO absorption bands are labeled. (b) Differential spectrum of the going bands are due to HNCO. Negative going bands belong to HCNO. (c) Spectrum of HNCO in Ne matrix. The HNCO bands are labeled.

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#### TABLE II

		HCNO			DCNO		
		Gas	Ne	Ar	Gas	Ne	Ar
۳s	δH(D)CN	224.6 <sup>a</sup>	239.2 <sup>a</sup>	243.0	163	b	b
		541.8	560.4	567.1	392.1	412.8	419.5
¥4	δCNO	537.3	539.1		-		-
¥3	₽5CNO	1254	1250.0	1244.2		1223.9	1218.1
¥2	cnoور	2196	2200.0	2193.2	2071	2072.7	2063.0
۳1	₽CH(D)	3336.1	3338.1	3317.8	2621	2625.3	2612.8
2 " 3	2498	2498	2492.2		-		
¥2+¥3			3429.7		-	3278.3	

Vibrational Transitions of Fulminic Acid in Solid Ne and Ar and Their Comparison with the Gas Phase (cm<sup>-1</sup>)

\* The accuracy of the matrix data is  $\pm 1$  cm<sup>-1</sup>.

<sup>b</sup>  $\nu_5$  for DCNO is below the range studied.

situation is similar also for the deuterated compound, with good agreement between the matrix frequencies and the gas phase data.

Of considerable interest are the two bending fundamentals, and in particular  $\nu_5$ , the bending mode of the HCN group. The HCN potential exhibits a small,  $\sim 12 \text{ cm}^{-1}$ , barrier to linearity (26), and the classical zero point vibrational amplitude is  $\pm 34^\circ$ . It is therefore interesting to examine the effect of the solid medium upon this high-amplitude hydrogen atom motion and upon the shallow, two-dimensional HCN bending potential surface. Winnewisser *et al.* (22) have examined the spectra of HCNO in solid *n*-hexane and HCN. They find that the spectrum is changed dramatically, and in particular, the value of  $\nu_5$  is almost doubled. They conclude that in the matrix, pronounced changes occur in the vibrational potential function and the observed spectrum is that of a linear molecule.

We find a quite different situation in the rare gas solids. The vibrational potential function of a quasilinear molecule is qualitatively unchanged and only relatively minor shifts in the vibrational levels are observed. It may be noted, however, that the levels associated with the HCN bending vibration  $\nu_5$  undergo somewhat larger relative shifts than the other vibrational modes.

Vibrational levels of  $v_5$  are described in terms of the limiting bent model by quantum numbers l and n. In the bent molecule limit, l becomes the rotational quantum number K and n the vibrational quantum number,  $v_5$  (bent), while in the linear molecule limit n becomes the angular quantum number with  $v_5$  (linear) = 2n + 1. In the 4 K matrix only the lowest l = 0, n = 0 level is populated, and selection rules permit transitions into the n = 0, l = 1 ( $v_5 = 1$ , II in the linear limit) and n = 1, l = 0 ( $\Sigma$  sublevel of  $v_5 = 2$  in linear limit) levels. These are observed in solid neon at 239 and 560 cm<sup>-1</sup>, respectively, slightly blue-shifted from their gas phase positions (224 and 542 cm<sup>-1</sup>). In solid argon they shift even further to 243 and 567 cm<sup>-1</sup>.

This situation is somewhat reminiscent of  $C_6F_6^+$  and similar cations in rare gas matrices, which exhibit Jahn-Teller distortions in their ground electronic states (32-34). While these species in general exhibit in solid neon negligibly perturbed spectra, the Jahn-Teller active modes, which are similarly characterized by a potential function with central maximum, also show in the more polarizable Ar and Kr solids larger relative matrix shifts than the other modes.

## ULTRAVIOLET SPECTRA

Several attempts were made to record the spectra of HCNO and HNCO in the ultraviolet and visible. The electronic spectra of both compounds have been previously studied in the gas phase. For HCNO a spectrum between 2850 and 2440 Å, consisting of a single progression of diffuse bands probably due to one of the bending frequencies was reported by Sheasley and Mathews (34). The HNCO spectrum extends, with gradually increasing intensities (35) from 2800 Å to beyond 2000 Å. Like that of the fulminic acid it shows evidence of extensive excitation of the upper state bending frequencies and of predissociation. The matrix work is complicated by the fact that exposure to the xenon arc radiation used to record the spectra leads to photolysis of both of the compounds studied. One thus observes that spectra of the photolysis products, CNO and NCO, grow in gradually. Also, diatomic fragments NH, OH, and CN appear in the photolyzed samples. From the rather limited data we could obtain, it appears that the matrix spectra of both compounds are broad and lack any vibrational structure. Their contours and positions agree relatively well with the reported gas phase studies. No lower-lying absorptions attributable to either of the two compounds were found.

#### HCNO PHOTOLYSIS AND ISOMERIZATION

As mentioned in the preceding section, when the samples of HCNO in neon are exposed to the unfiltered radiation of a 50-W Xe arc, a very fast decrease in the intensity of the HCNO bands is observed. One of the advantages of using our FTIR instrument is that data are obtained in digital form. One can thus readily use spectral subtraction techniques to identify clearly the effects of sample photolysis. An example of such a subtracted spectrum showing the effects of exposure of HCNO + Ne (1:5000) sample for 10 min to the unfiltered Xe arc radiation is presented in Fig. 1b. Here the negative going peaks, indicative of decreasing absorbance, are due to HCNO. On the other hand, most of the stronger positive going bands are identified as growing absorptions of the HNCO photoproduct, showing that isomerization to isocyanic acid is the major process.

In addition, a few moderately strong absorptions at 3610, 2294, 1227, and 1082  $cm^{-1}$  also grow in intensity with time. These are not HNCO bands, since they do not appear in the spectrum of directly deposited HNCO. If, however, a pure HNCO sample in neon is photolyzed by the xenon arc one observes that the HNCO absorptions now decrease, although rather slowly, while the above four bands again





FIG. 2. Schematic diagram showing the energetics of CHNO isomerizations and the photoprocesses occurring in the matrix. The relative energies of the individual isomers and the barrier heights were compiled from the theoretical works in Refs. (6-8).

become stronger. They are undoubtedly the same bands observed by Jacox and Milligan (27) following 1216 Å photolysis of HNCO in solid Ar at 3572, 2288, 1228, and 1080 cm<sup>-1</sup>. Their appearance in the present experiments confirms their assignment to HOCN, cyanic acid. In experiments with deuterated fulminic acid in neon the HOCN bands shift to 2664, 2792, 948, and 1077 cm<sup>-1</sup>, respectively. A fifth fundamental of HOCN reported by Jacox and Milligan (27) at 460 cm<sup>-1</sup> in solid Ar (437 cm<sup>-1</sup> in the deuteride) was not detected in the present experiments and is apparently much weaker than the other bands.

The absorptions of cyanic acid appear to grow in concurrently with the isocyanic acid bands when HCNO is photolyzed. Furthermore, the rate of growth of these absorptions under otherwise similar conditions is greater when fulminic acid samples are irradiated than for photolysis of isocyanic acid. We therefore conclude that cyanic acid is formed directly as a by-product of the fulminic acid photolysis and not by secondary photolysis of the isocyanic acid product.

We have examined briefly the rate of fulminic acid photolysis as a function of wavelength. There appears to be no observable photolysis for  $\lambda > 2900$  Å. With a 2800-Å cutoff filter, slow photolysis is observed and the rates increase at shorter wavelengths. This suggests that the photolytic efficiency simply follows the

absorption spectrum of fulminic acid, which shows an onset near 2850 Å in the gas phase.

Our studies do not permit us to determine with confidence the mechanism of the rearrangement. The uv transition of fulminic acid is rotationally diffuse (34), presumably due to predissociation of the excited electronic state. The fact that dissociation into H + CNO does, at least to some extent, occur in the matrix was confirmed by the observation of the CNO visible absorption spectrum following hydrogen or xenon lamp photolysis (1). If the main predissociation channel involves  $HCNO \rightarrow H + CNO$ , one might expect isofulminic acid, HONC, to form as one of the major products. Yet, no evidence of isofulminic acid was found, even though it is predicted to be stable and separated by a fairly high barrier from its isomers. One possibility might be that the HCNO predissociation forms CNO in an excited electronic state. We have shown recently (1) that CNO possesses a low-lying electronic state near 1.5 eV, and that nonradiative relaxation of this state leads to rearrangement to NCO with high, probably near unity, quantum yield. In this way, the reaction path would be

> HCNO + h $\nu$  → H + CNO\*(Å), CNO\*(Å) → NCO(X), NCO(X) + H → HNCO or NCOH.

Such recombination of NCO with a hydrogen atom would explain the formation of cyanic and isocyanic acid, as well as the absence of isofulminic acid. A feasibility of this channel does require a fairly low C-H bond energy in the excited state of HCNO (<65 kcal/mole). Alternatively, the initial dissociation step may lead to HCN + O. This reaction channel is apparently energetically also accessible. Indeed, the lowest energy pathway from fulminic acid to HNCO is predicted to proceed via an oxazirine ring intermediate, resembling HCN bound very loosely to the oxygen atom (8).

One can also imagine the isomerization as proceeding without "dissociation" during the fast nonradiative relaxation of excited HNCO states. The HNCO electronic spectrum is known to exhibit a long vibrational progression involving probably the CNO bending frequency, suggesting a strongly bent excited state. During the nonradiative relaxation of this bent excited state, the ground-state bending modes will undoubtedly be strongly excited and rearrangement to HNCO (or HOCN) can take place. The barrier for isomerization into isofulminic acid is predicted to be considerably higher, and this may explain the absence of any evidence for HONC in our spectra.

The energetics of the CHNO isomerizations and the photoprocesses observed in rare gas matrices are summarized in Fig. 2. It is interesting to note that isomerization of HNCO samples in the opposite direction, to yield HCNO, did not occur even though it is energetically possible for photolysis with the Lyman- $\alpha$  hydrogen line (1216 Å) and with the rare gas atomic resonance lines. Even after several hours of photolysis of HNCO, HOCN and the NCO free radical were the only products observable in the infrared spectrum.

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#### PYROLYSIS OF ISOXAZOLONES AND HCNO FORMATION

A convenient preparation of fulminic acid was recently developed by Briehl and co-workers (29). It involves thermolysis of 4-phenyl isoxazolinedione monoxime (I) according to the reaction

$$\begin{array}{c} C_{6}H_{5} & \searrow & N-O_{1} \\ C_{7}C & \longrightarrow & H \\ H_{1} & & \searrow & CO_{2} + C_{6}H_{5}CN + (CNOH) \end{array}$$
(1)

While, by analogy with similar reactions, isofulminic acid would be expected, its tautomer HCNO is found to be produced instead. Since it is not clear whether proton migration occurs during the fragmentation process or isomerization of initially produced CNOH takes place during the subsequent handling, we have briefly examined this pyrolysis directly using matrix isolation techniques. Material (I) was sublimed at a temperature of 100-120°C, passed through a heated quartz tube and codeposited in our cryostat with a large excess of Ne. The results are summarized in Table III. With the quartz pyrolysis tube heated near 400°C, fulminic acid was the major product, and strong CO<sub>2</sub> bands at 2348 and 668 cm<sup>-1</sup> also appeared. Numerous weaker bands were clearly due to benzonitrile. Strongest among these were at 561, 690, 759, 1030, 1072, and 2230 cm<sup>-1</sup>, in good agreement with the published spectra (36). Several additional bands which cannot be associated with any of the products expected based on Eq. (1) appeared, the strongest of these being at 1829 cm<sup>-1</sup>. When the sample is exposed to xenon arc radiation, the 1829cm<sup>-1</sup> line disappears rapidly, while the HCNO absorptions disappear at a slower rate. At the same time one observes a growth in the isocyanic acid absorptions. Several other absorptions labeled "A" in Table III seem to decrease at a similar rate as the 1829-cm<sup>-1</sup> line, and may be due to the same absorber.

When the sample is deposited with the secondary furnace at  $\sim 200^{\circ}$ C, a very complex spectrum is observed. In addition to the CO<sub>2</sub>, benzonitrile, HCNO, and absorber "A," numerous new bands labeled "B" in Table III appear. The 1829-cm<sup>-1</sup> "A" absorption is now the strongest band in the spectrum. When this sample is exposed to Xe arc radiation, all the "B" absorptions are completely destroyed in less than 10 min, suggesting a very photolytically unstable compound. The HCNO bands and the "A" absorptions disappear at a much slower rate. On the other hand, one observes a growth of the absorptions of CO<sub>2</sub>, HNCO, and benzonitrile.

While, in the absence of isotopic information, it is difficult to make confident assignments, it is interesting to speculate on the identity of absorbers "A" and "B." The spectrum of the "B" compound is very similar to that of the starting compound in a KBr pellet, and it is very likely due to matrix isolated (I).

The spectrum of "A" is simple and it is undoubtedly due to a smaller molecule. It is enticing to propose that it could be the isofulminic acid. The prominent 1829- $cm^{-1}$  band lies in a relatively unusual frequency range. The frequency is somewhat low for the antisymmetric CNO stretch, but perhaps not unreasonably so if one considers that HONC is less stable than the other isomers and the bonding may

#### TABLE III

Vibrational Transitions	$(cm^{-1})$	) of the H	<b>Pyrolysis</b>	Products of	Isoxazolones	Codeposited	with Neon
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ν	assign.	Ī	assign	v	assign.
3782.7	H <sub>2</sub> O	1580.8	A	890	
3429.7	HCNO			881.5	в
3338.1	HCNO	1	C6H3CN	846.8	Α
25	HCNO	1452.5	C₀H₅CN	772	
2347.5	CO <sub>2</sub>	1400.0			
2268.4	HNCO	1374.4	A	759.0	C <sub>6</sub> H <sub>5</sub> CN
2200.0	HCNO	1250.0	HCNO	690.6	C <sub>6</sub> H <sub>5</sub> CN
2140	CO	1218.1	A	670	CO <sub>2</sub>
1829.6	В	1154.5	в	664.5	Α
1808.4	Α	1100	A	644.3	В
1758.2	Α	1077.3	A <b>€</b> 6H5CN		
1630.9	H <sub>2</sub> O	1053.2	A	539.1	C <sub>6</sub> H <sub>5</sub> CN
1614.5	H <sub>2</sub> O	940	A	302.8	A
1599.1	C <sub>6</sub> H₅CN	907.6	в		

thus be weakened. A weaker band near  $1155 \text{ cm}^{-1}$  could then be the symmetric CNO stretch. Alternatively, "A" could be a larger intermediate, possibly involving CNOH and CO<sub>2</sub>. Further work, including isotopic substitution studies, would clearly be desirable.

### SUMMARY

Ultraviolet photolysis of HCNO in solid Ne leads to efficient isomerization to HNCO, with NCOH being a minor ( $\sim 15\%$ ) by-product. The NCO radical appears to be the major fragment product for either of the CHNO species. Its isomer CNO, while observable in the visible, was not stabilized in concentrations sufficient for infrared detection.

RECEIVED: October 30, 1981

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