DETECTION OF MOLECULAR MICROWAVE TRANSITIONS IN THE 3 MM WAVELENGTH RANGE IN COMET KOHOUTEK (1973f)

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Introduction

We have recently reported detection of hydrogen cyanide and

the first quantitative observations of the velocities of neutral

gas jets in the inner part of the coma while the comet was at

small heliocentric distances (Huebner, et al., 1974). Now we report

the detection of two line transitions from unidentified cometary

molecules, provide further evidence of the variability of neutral

gas jets, and give a summary of our search program for microwave

transitions in molecules of cometary origin.

The observations presented here were made with a 3-mm line

receiver mounted on the 11-m NRAO** radio dish at Kitt Peak. Observa-

tions were carried out before perihelion (15 to 20 December 1973)

and after perihelion (3 to 7 January 1974). During these periods

the comet was between 0.3 and 0.5 AU heliocentric distance. The

antenna half-power beam width at 3 mm wavelength is $\theta_B \approx 80$ arc s.

The observations are based on data obtained from filter banks with

a resolution of 250 kHz and 100 kHz. Small local oscillator frequency

offsets were made to check for system-generated signals. Searches

at off-comet positions were carried out to obtain comparison spectra

for noise determination. Comet velocity and position was obtained

from ephemerides calculated independently by T. Clark (Goddard Space

Flight Center) and Rh. Lüst (Max-Planck-Institut für Astrophysik,

Munich). The two sets of ephemerides agreed to within the pointing accuracy (10 arc s) of the telescope.

Table 1 summarizes the observational data. The columns, in order, list the UT date of observation, average comet position (RA and Dec) during each period of observation, molecular transition searched for, total integration time (δt), single-sideband r.m.s. system temperature (T_S^*) obtained from all calibrations made during the integration interval, heliocentric distance (r) of the comet, geocentric distance (Δ) of comet, geocentric radial velocity component ($\dot{\Delta}$) of comet, and the rest frequency (ν_o) of the theoretically strongest component of the molecular transition.

Hydrogen Cyanide

The detection of HCN has been reported earlier (Huebner, et al., 1974). Here we present the spectral data of the $H^{12}C^{14}N$ J = 1 - 0 transition with more time resolution to show the variability of the gas jets and consistency of this phenomenon in other mother molecules. Figure 1(A) illustrates the average composite spectrum obtained December 15 and 16. In Figs. 1(B) and 1(C) the same transitions are presented as observed on January 3 and 6. The bars above each spectrum indicate the frequencies of the three hyperfine quadrupole components F = 0 - 1, 2 - 1, and 1 - 1, belonging to the same Doppler shifted velocity group measured with respect to the rest frame of the comet's nucleus. These laboratory frequencies as measured by DeLucia and Gordy (1969) are 88.63394 GHz, 88.63185 GHz, and

TABLE 1

Observational Data

| UT Date	Comet (1950) RA [h m]	Dec [° ']	Transition	ΔT_{pp} [K]	r [AU]	Δ [AU]	$\dot{\Delta}$ [km/s]	ν_0 [GHz]
Dec 15.8	15 41.4	-25 41	HCN (1-0)	--	.49	1.16	-12.5	88.631847
Dec 16.7	15 51.4	-25 51	CH_3CN (v_8=1,5_K-4_K)	--	.46	1.15	-10.5	92.261440
Dec 16.8	15 52.5	-25 52	HCN (1-0)	--	.46	1.15	-10.3	88.631847
Dec 17.7	16 02.9	-25 58	CH_3CN (v_8=1,5_K-4_K)	--	.43	1.14	- 8.3	92.261440
Dec 17.8	16 04.1	-25 59	CH_3CN (v_8=1,5_K-4_K)	--	.43	1.14	- 8.0	92.261440
Dec 17.9	16 05.3	-26 00	X-ogen	0.5	.43	1.14	- 7.8	89.189
Dec 18.6	16 13.6	-26 03	X-ogen	0.2	.40	1.14	- 6.2	89.189
Dec 18.6	16 13.6	-26 03	CH_3CN (5_K-4_K)	--	.40	1.14	- 6.2	91.98705
Dec 18.7	16 14.8	-26 03	HNC (1-0)	0.3	.40	1.14	- 6.0	90.665
Dec 18.7	16 14.8	-26 03	HNCO (4_{04}-3_{03})	0.3	.40	1.14	- 6.0	87.92524
Dec 18.8	16 16.0	-26 03	CH_3C_2H (5_K-4_K)	0.4	.40	1.14	- 5.8	85.45729
Dec 18.8	16 16.0	-26 03	HNCO (4_{13}-3_{12})	0.4	.40	1.14	- 5.8	88.23905
Dec 18.9	16 17.2	-26 03	HCN ($2v_2$,1-0)	0.7	.40	1.14	- 5.6	89.08792
Dec 19.7	16 27.1	-26 03	HCN ($2v_2$,1-0)	0.3	.37	1.14	- 3.8	89.08792
Dec 19.8	16 28.3	-26 03	CH_3CN (v_8=1,5_K-4_K)	--	.37	1.14	- 3.6	92.261440
Dec 20.7	16 39.8	-25 59	HC_3N (10-9)	0.4	.34	1.14	- 1.6	90.981
Jan 3.9	20 07.6	-16 42	HCN (1-0)	--	.30	0.94	-41.8	88.631847
Jan 4.8	20 18.4	-16 00	SiO (v=1,2-1)	0.3	.33	0.92	-38.3	86.24328
Jan 4.9	20 19.6	-15 55	$(CH_3)_2O$ (2_{20}-2_{11})	0.4	.34	0.92	-37.9	86.22804
Jan 4.9	20 19.6	-15 55	SiO (v=1,2-1)	0.4	.34	0.92	-37.9	86.24328
Jan 5.0	20 20.8	-15 51	SiO (v=1,2-1)	0.3	.34	0.92	-37.5	86.24328
Jan 6.8	20 42.2	-14 22	HCN (1-0)	--	.39	0.88	-30.6	88.631847
Jan 6.9	20 43.4	-14 17	SiO (v=1,2-1)	0.8	.40	0.88	-30.1	86.24328
Jan 7.0	20 44.6	-14 12	SiO (v=1,2-1)	0.3	.40	0.88	-29.8	86.24328
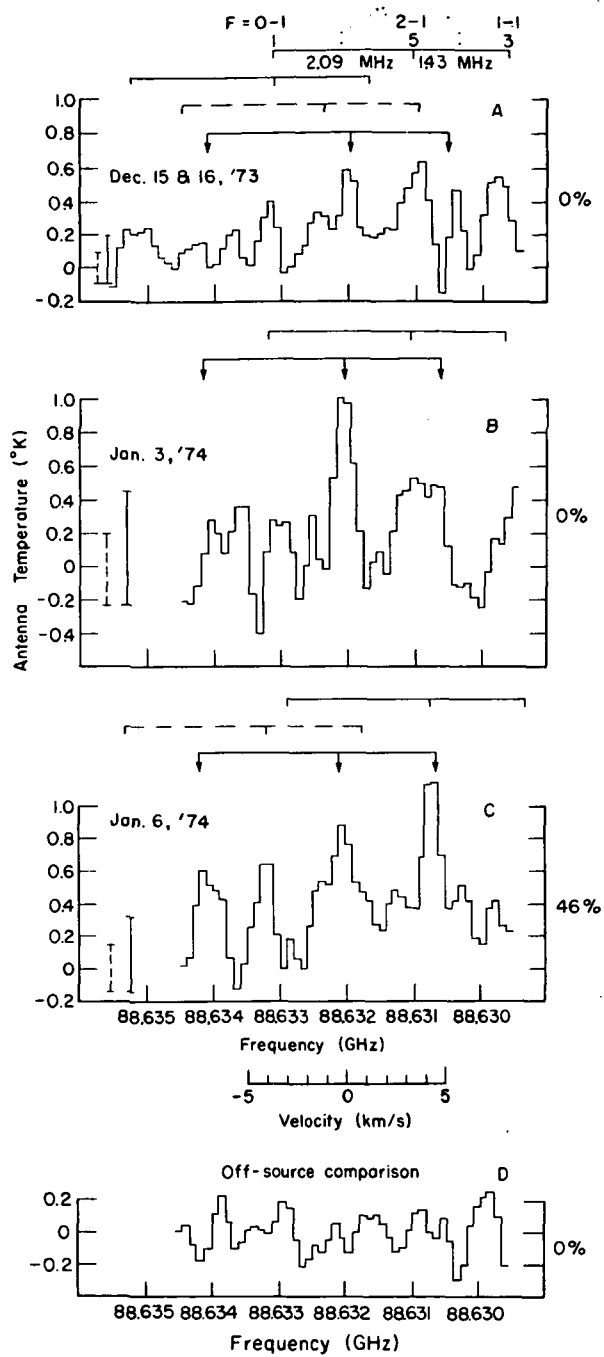
Figure 1: Emission spectrum of the HCN J = 1-0 transition observed in comet Kohoutek (1973 f) before perihelion (A) and after perihelion (B) and (C).

88. 63042 GHz. Within each group the observed intensities follow

closely the predicted theoretical values (2F + 1) indicated above

the top bar. The triplet with zero Doppler shift (within the width

of a channel) with respect to the nucleus is indicated by arrows.

It appears to be present in each spectrum, but fluctuates with time.

The intensity of the other triplets also fluctuates with time, but

in addition they change their number and frequency shift. The

transitions with zero Doppler shift can be interpreted as a

quiescent outstreaming of slowly released gas, however, their time

variation suggests that they are also outbursts with velocities

consistent with the other Doppler shifts, but close to the plane

perpendicular to the earth-comet direction. There is no discernable

decrease of intensity in the post-perihelion observations. Only the

strongest Doppler shifted components of the spectrum are identified,

possible weaker ones are indicated by dashed bars. Doppler shifts

up to ∼1.3 MHz (∼4 kms^{-1}) can be measured. Figure 1(D) is a spectrum

taken while tracking ∼7.5 arc min <u>off</u> the comet nucleus and was

used to determine the peak-to-peak noise which was found to be ∼0.3°K.

The peak-to-peak noise is indicated by two error bars in Figure 1. The

dotted error bar indicates the noise with the dome open, the solid error

bar indicates the increase in noise due to dome attenuation. The per-

centage of time during which observations were made with the dome open

is given to the right.

Methyl Cyanide

Following the unexpected detection of $^{12}CH_3^{12}C^{14}N$ in its $v_8 = 1$

excited state, transition $J_K = 6_3 - 5_3$ by Ulich and Conklin (1974)

on 1 and 5 December, 1973, we searched for the next lower rotational

transition in the same vibrational state on 16, 17, and 19 December.

Although signals 3 to 4 times peak-to-peak noise were detected

in the 100 kHz filter bank the variability in intensity and frequency

of the Doppler shifted lines resulted in identification problems:

Doppler shifts similar to those measured in HCN could also be infered

in the CH_3CN spectrum, but since the spacing of its K-component

lines is bigger than the hyperfine splitting of the HCN spectrum

one or the other of two K-components was frequently shifted out of

the range of the 100 kHz filter bank. For this reason we present

the analysis of the CH_3CN spectrum in the 250 kHz filter banks.

The average of the spectra obtained by Ulich and Conklin on

1 and 5 December with the 100 kHz filter banks are presented in

Fig. 2(A). The frequency scale has been reversed to facilitate

comparison of their observation of the $J_K = 6_0 - 5_0$ and $6_3 - 5_3$

transition with our $J_K = 5_0 - 4_0$ and $5_3 - 4_3$ observations.

Figure 2(B-D) presents our observed spectrum of $^{12}CH_3^{12}C^{14}N$ in

the $v_8 = 1$ excited state. The transitions correspond to $J_K = 5_2 - 4_2$,

$5_0 - 4_0$, $5_3 - 4_3$, and $5_1 - 4_1$. The corresponding frequencies as

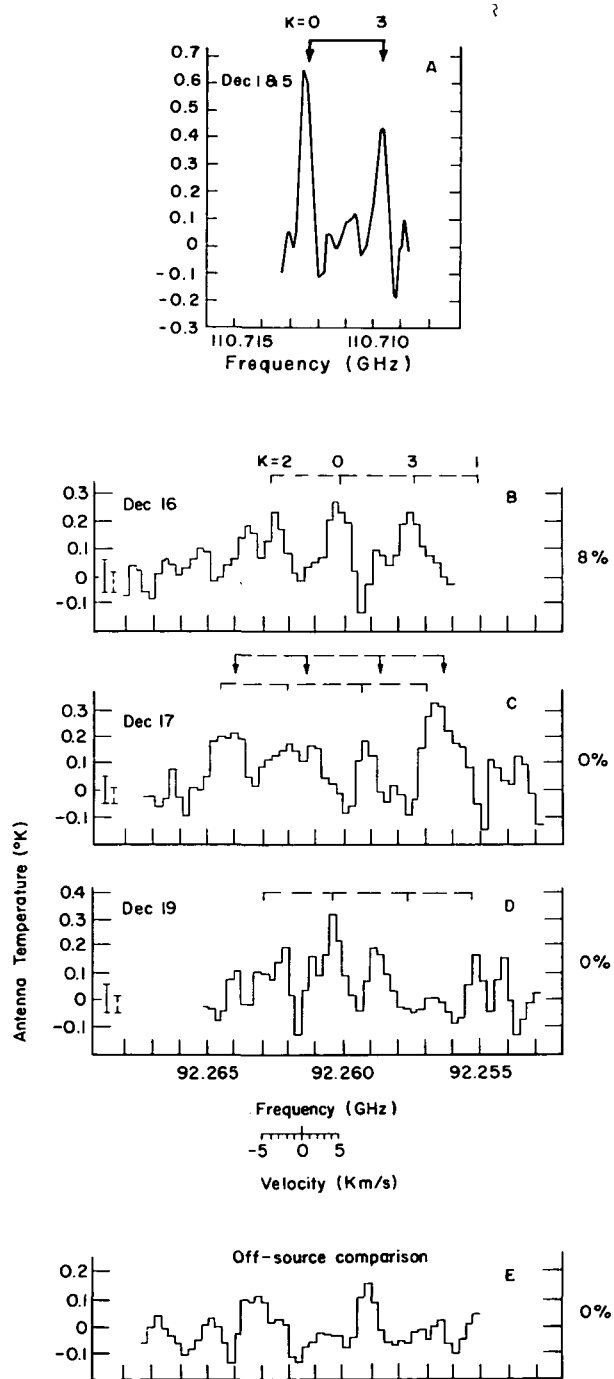measured by Bauer and Maes (1969) are 92.26399 GHz, 92.26144 GHz,

Figure 2: Emission spectrum of the CH_3CN $v_8 = 1$ state observed in the comet in the $J_K = 6_0 - 5_0$ and $6_3 - 5_3$ transitions (A) and the $J_K = 5_K - 4_K$, $K = 0$, 1, 2, and 3 transition (B), (C), and (D).

92.25841 GHz and 92.25629 GHz. Doppler shifts up to about ± 1.0 MHz are measured. The zero point of the velocity scale below Fig. 2(D) indicates the expected position of the K = 0 component under quiescent conditions. Bars above each spectrum connect K-components exhibiting the same Doppler shift; the bar with arrows pointing downward indicates transitions of the "quiescent" state with nearly zero Doppler shift. It should be noted that the "quiescent" state is not always present, which strengthens the interpretation that it is due to jets in a plane perpendicular to the line of sight rather than a uniform out-gassing. The spectra as presented in Fig. 2(A-D) get progressively weaker. Only our 16 and possibly 17 December spectra are strong enough to serve as confirmation of the detection of CH_3CN by Ulich and Conklin. The signal to noise ratio is insufficient for a direct and independent identification of the molecule.

On 18 December we made a search for $^{12}CH_3^{12}C^{14}N$ vibrational ground state $J_K = 5_K - 4_K$ transitions simultaneously with a search for X-ogen (Buhl and Snyder, 1970) in the other side-band of the receiver. There was a possible detection of weak components $(|K| = 3, 2, 0,$ and $1)$ at about $T_A^* = 0.4$K. The corresponding rest frequencies measured by Bauer and Maes (1969) are 91.97137 GHz, 91.98000 GHz, 91.98528 GHz and 91.98705 GHz.

Two unidentified lines

On 3 January Snyder and Buhl (1974) discovered a peculiar masering transition with several frequency components as a point source

in Orion. A search for these lines was made in the comet on 4,5,6, and 7 of January with several shifts of the local oscillator frequency. As a result of this search two lines were acquired one in the upper side-band of the 250 kHz filter bank receiver at 89.0105 GHz and one in the lower side-band at 86.2471 GHz. The summary of these observations is presented in Fig. 3(A and B). The interstellar lines were later identified as Doppler shifted components of SiO with rest frequency 86.24328 GHz corresponding to the transition $v = 1$, $J = 2 - 1$ (Snyder and Buhl, 1974) and cannot be brought into agreement with the lines observed in the comet. There are no known transitions in the neighborhood of 89.0105 GHz. The frequency of the other line (86.2471 GHz) is close to that of ethanol (86.2474 GHz) and acetone (86.2479 GHz), but probably cannot be identified with either one of these molecules for the following reasons: (A) The line is too broad, indicating an approximately isotropic expansion velocity of ~ 3 kms^{-1}. This requires the additional assumption that an exothermic process took place. (B) The line does not exhibit the resolvable Doppler shifted components and thus is not consistent with the HCN and CH_3CN observations made at about the same heliocentric distance. (C) If the molecule were acetone one would also expect to find a line at 86.2447 GHz which is not observed. The source of the two unidentified lines is probably a radical which during the process of decay of its mother molecule received an excess of kinetic energy as, e.g., can occur during photodissociation.
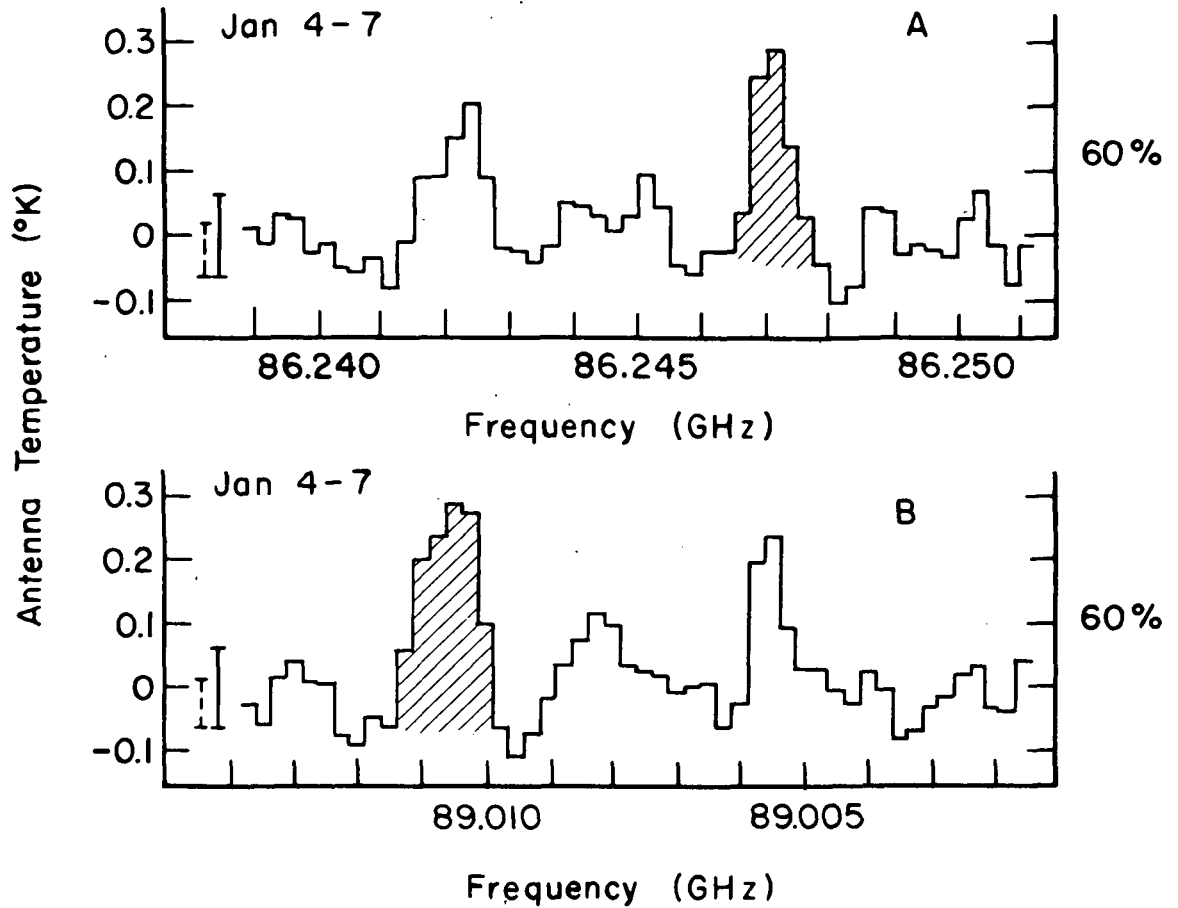
Fig. 3. Two unidentified line transitions found during the Si 0
search in the lower side band (A) at 86.2471 GHz and
in the upper side band (B) at 89.0105 GHz. Since lower and
upper side band of the receiver are super imposed in the
display but with frequencies increasing in opposite direc-
tions the line transitions show up in both spectra (A) and
(B) but the side band to which they belong can be assigned
uniquely through shifts in the local oscillator frequency.

Production Rates

Figure 4 presents the earth's orbit and the projection of the comet's orbit on the ecliptic and indicates the times and heliocentric distances when the above-mentioned observations were carried out. Ulich and Conklin observed between 1 and 5 December when the comet was at heliocentric distances between 0.87 and 0.79 AU. Their spectra indicate a quiescent production of methyl cyanide. Our observations of methyl cyanide were made when the comet was between 0.46 and 0.37 AU heliocentric distance before perihelion. By that time the production was very weak and getting weaker. Discrete jets with speeds of several km/sec with respect to the nucleus are measured from Doppler shifts. These indicate an inhomogeneous struc-ture of the nucleus (Huebner, 1974, 1975). Observation of the spectrum in the vibrationally excited state $\sim$640 $^{\circ}$K above the ground state, the lack of a Boltzmann distribution, and the action of jets make estimates for the abundance very difficult. In the absence of detailed knowledge about the excitation mechanism and the cross sectional area of the jets we apply a quiescent state fluid dynamic model (Huebner and Snyder, 1970) to our ground state observation.

The fluid model is valid as long as:

$$A < n \, v\sigma \tag{1}$$

where A = Einstein emission coeff. for microwave transition in sec^{-1}, n = number density of molecules/cm^3, v = escape velocity $\approx$ thermal velocity $\approx 3 \times 10^4$ cm/sec and σ = collision cross section $\approx 10^{-15}$ cm^2.
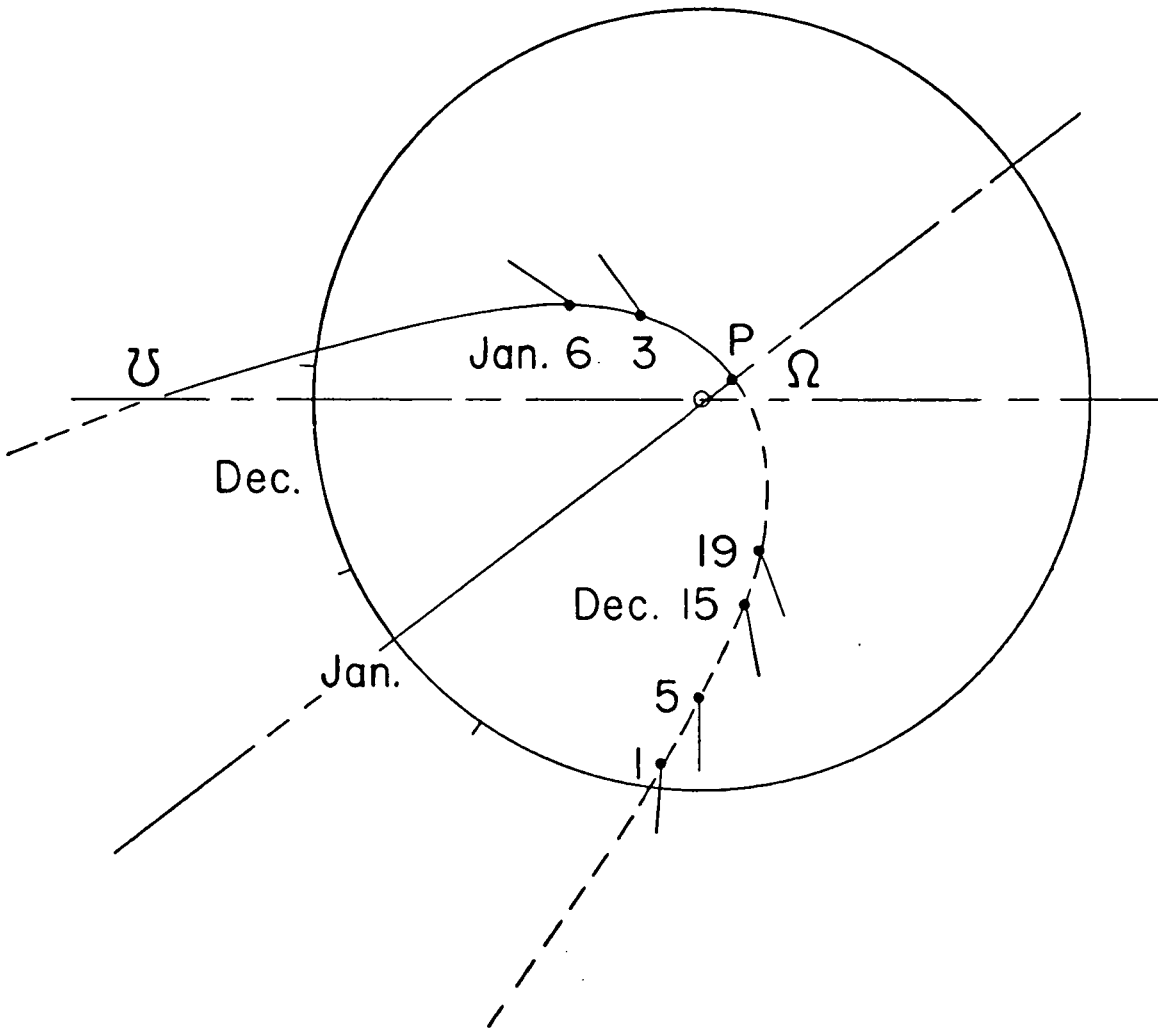
Fig. 4. Projection of the orbit of the comet onto the ecliptic. Earth positions for December 1, January 1, and February 1 are indicated on the circle. Comet positions corresponding to the dates of observations by Ulich and Conklin and by us are shown on the parabola.

For our fluid dynamic model

$$n = \frac{Z}{v} \left(\frac{R}{r}\right)^2 \qquad (2)$$

Where Z = gas production rate of comet $\approx (10^{18}/r_h{}^2)$ molecules sterad^{-1} cm^{-2} sec^{-1} for $r_h \leq 1$ AU where r_h = heliocentric distance in AU; R = radius of nucleus ≈ 3 to 5×10^5 cm for Kohoutek, and r = radial distance of molecules in the coma as measured from center of nucleus.

$$\therefore \quad A < \frac{Z \sigma}{r_h{}^2} \left(\frac{R}{r}\right)^2 \approx (10^{18}/r_h{}^2) \times 10^{-16} (10^{5.5}/r)^2$$

$$\qquad (3)$$

$$A < 10^{13}/(r r_h)^2$$

In our calculations $r_h \approx 0.3$ to 0.5 AU. We assumed two cutoff values for r: $r_o = 10^4$ km $= 10^9$ cm and $r_o = 10^5$ km $= 10^{10}$ cm.

$$\therefore \quad A < 10^{-3} \text{ sec}^{-1} \text{ for } r_o = 10^4 \text{ km} \qquad (4a)$$

$$A < 10^{-5} \text{ sec}^{-1} \text{ for } r_o = 10^5 \text{ km} \qquad (4b)$$

The fluid model breaks down when the collision mean free path becomes larger than the distance traveled, i.e., it breaks down at $r \approx 1/(n\sigma)$, or $r \approx Z R^2 \sigma/v \approx 10^{10}$ cm. Hence, within the cutoff radius which we consider the fluid model is valid.

The optical depth, frequency-averaged over the full width ($\Delta \nu$) of a line at one-half the maximum line intensity, for a symmetric top

molecule is

$$(\tau) = \frac{16\pi^2 \langle N \rangle \, f_v \, h^{3/2} \, \mu^2 \, \nu^2 \, (ABC)^{1/2}}{3c \, \Delta\nu \, (kT)^{5/2}} \cdot \frac{(J+1)^2 - K^2}{J+1} e^{-W/T},$$

$$(5)$$

for $(J+1)_K \rightarrow J_k$.

The effects of beam dilution, β, have been included, i.e.,

$$\langle \tau \rangle \equiv \beta \bar{\tau} , \qquad (6)$$

and

$$\langle N \rangle \equiv \beta N . \qquad (7)$$

Here N is the column density of the total number of CH_3CN molecules, μ is the dipole moment (3.92×10^{-18} esu·cm for CH_3CN), ν is the transition frequency, and A, B, and C are the rotational constants (A = B = 9.199 GHz, C = 158.0 GHz and CH3CN). The rotational energy of the upper level W = 13.2 $^{\circ}K$ for $J_K = 5_0 - 4_0$ in CH_3CN enters the assumed Boltzmann distribution for the vibrational ground state for which the partition function is $f_v \approx 1$.

If the comet coma is optically thin and its 3 mm continuum emission is negligible then the antenna temperature, T_A^*, as measured by chopper wheel calibration is related to the optical depth, Eq. (5), by

$$T_A^* = T \langle \tau \rangle . \qquad (7)$$

If emission is not enhanced (which is apparently not true for the $v_8 = 1$ state) by collisional or radiative excitation, then the

temperature is determined by the vaporization equilibrium, $T \approx 150$ $^{\circ}$K.

An upper limit for the K = 0 component is $T_A^* \approx 0.4$ $^{\circ}$K. This gives for

the optical depth including beam dilution $\langle \tau \rangle \approx 0.0027$. Although

smoothing gives the lines a much broader appearance, the total half-

intensity line width $\Delta \nu \approx 200$ kHz. Substitution into Eq. (1) gives

for the column density including beam dilution $\langle N \rangle \approx 1.6 \times 10^{13}$ cm^{-2}

as an approximate upper limit. The range of the methyl cyanide

molecules before they are destroyed by photodissociation or photo-

ionization is not known. Two typical values will be assumed for the

cutoff range, $r_o = 10^4$ and 10^5 km. The column density uniformly

distributed over the antenna beam is

$$\langle N \rangle = \frac{4Q'}{\pi v \Delta^2 \theta_B^2} \left[s \cos^{-1} \frac{s}{r_o} - (r_o^2 - s^2)^{1/2} + r_o \right] \tag{9}$$

with

$$s = \min[r_o, \Delta \cdot \theta_B/2]. \tag{10}$$

Here Q' is the total production rate of the molecule under consideration,

$v \approx 0.3$ kms^{-1} is the average (thermal) expansion velocity of the escaping

gas, θ_B is the half-power antenna beam width, and Δ is the geocentric

distance of the comet. Using $\Delta = 1.14$ AU an upper limit for the produc-

tion rate of CH$_3$CN at r = 0.40 AU heliocentric distance is Q' = 1.7 $\times$

10^{28} s^{-1} for $r_o = 10^4$ km and Q' = 3.6 $\times$ 10^{27} s^{-1} for $r_o = 10^5$ km.

The production rate of HCN based on observations of the J = 1-0

vibrational ground state transitions was reported earlier by Huebner,

et al., (1974) to be $Q' = 1.2 \times 10^{28}$ s^{-1} for the cutoff range $r_o = 10^4$ km and $Q' = 3 \times 10^{27}$ s^{-1} for $r_o = 10^5$ km. No spectrum could be detected in the vibrationally excited 2ν state. Upper limits for production rates of other molecules listed in Table 1 can be obtained, taking into account the appropriate molecular symmetry properties in the calculation of the optical depth (see, e.g., Townes and Schawlow, 1955). The results are summarized in Table 2.

Production rates are related to abundances of the constituents in the frozen state, but latent heats of vaporization and likely inhomogenities in the structure of the nucleus must be considered in such an analysis. It should be noted that, with the sole exception of water, only molecules with strong transition probabilities in the radio range have been detected. Other molecules may be more abundant, yet their detection is more difficult because of weak transition probabilities or high latent heats of vaporization. The difficulties encountered with the detection of water by Jackson, et al., (1975) is a typical example.

Table 2

Summary of Production Rates, Q', and Related Quantities

Molecule	T_A^* [°K]	$<\tau>$	A [s⁻¹]	$<N>$ [cm⁻²]	Q' [s⁻¹] for $r_o=10^4$ km	$r_o=10^5$ km
HCN (1-0)	0.8	0.0054	2.4×10^{-5}	1.5×10^{13}	1.2×10^{28}	3×10^{27}
CH_3CN (5_K-4_K)	0.4	0.0027	9.4×10^{-5}	1.6×10^{13}	1.6×10^{28}	4×10^{27}
X-ogen	<0.3					
HNC (1-0)	<0.3	<0.002				
HNCO (4_{04}-3_{03})	<0.3	<0.002	8.9×10^{-6}	$<4 \times 10^{13}$	$<5 \times 10^{28}$	$<1 \times 10^{28}$
CH_3C_2H (5_K-4_K)	<0.4	<0.003	2.8×10^{-6}	$<3 \times 10^{15}$	$<3 \times 10^{30}$	$<1 \times 10^{30}$
			6.3×10^{-5}			
HC_3N (10-9)	<0.4	<0.0025	2.9×10^{-5}	$<3 \times 10^{12}$	$<4 \times 10^{27}$	$<1 \times 10^{27}$
Si O (v=1,2-1)	<0.1	<0.001	2.2×10^{-6}	$<7 \times 10^{16}$	$<6 \times 10^{31}$	$<2 \times 10^{31}$
$(CH_3)_2O(2_{20}$-$2_{11})$	<0.4	<0.003				

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