The detection of hot ethanol in G34.3+0.15

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ABSTRACT
Hot molecular cores in star-forming regions are known to have gas-phase chemical compositions determined by the evaporation of material from the icy mantles of interstellar grains, followed by subsequent reactions in the gas phase. Current models suggest that the evaporated material is rich in hydrogenated species, such as water, methane and methanol. In this paper, we report the detection of 14 rotational transitions of ethanol in the submillimetre spectrum of the molecular cloud associated with the ultra-compact H II region G34.3+0.15. We derive a rotation temperature of 125 K and a beam-averaged column density of 2.0×10^{15} cm^{-2}, corresponding to a fractional abundance on the order of 4×10^{-9}. This large abundance, which is a lower limit due to the likelihood of beam dilution, cannot be made by purely gas-phase processes, and we conclude that the ethanol must be formed efficiently in the grain surface chemistry. Since it has been argued previously that methanol is formed via surface chemistry, it appears that alcohol formation may be a natural by-product of surface reactions.

Key words: molecular processes – ISM: clouds – dust, extinction – ISM: molecules – radio lines: ISM.

1 INTRODUCTION

Ethanol, CH_3CH_2OH, was first detected in Sgr B2 by Zuckerman et al. (1975). Since then, several different detections have been made in the Sgr B2 cloud, but, with the exception of detection in W51M by Millar et al. (1988), ethanol has proved elusive. The spectral scans of Orion-KL by Johansson et al. (1984) at 3 mm, and by Blake et al. (1987) at 2 mm failed to detect it. Turner (1991) has claimed identification in Orion from his spectral scan at 70–115 GHz, but Ziurys & McGonagle (1993) have not detected it at 2 mm. Most recently, Ohishi (private communication) has detected it in several hot core sources. The excitation and abundance are not well known, in part due to the uncertainty concerning the detection of weak a-type transitions, for which $\mu_a = 0.046$ Debye, which are a factor of ≈ 1000 weaker than the b-type transitions with $\mu_b = 1.438$ Debye. The rotational energy levels are designated J_{K-K+}. The b-type transitions link energy levels of either even or odd parity, i.e. K– + K+ = even ↔ even or odd ↔ odd, respectively, while the a-type transitions connect even ↔ odd. In this paper, we present JCMT observations of several transitions of ethanol in the 330–360 GHz range toward the molecular cloud surrounding the ultra-compact H II region G34.3+0.15. The frequencies are taken from an extensive laboratory and theoretical study by Pearson et al. (1995) and are accurate to within 1–2 MHz. Since we have detected several transitions, all of which are b-type, we can construct an accurate rotation diagram and derive a rotational temperature and column density.

2 OBSERVATIONS

The observations were carried out in 1991 July and 1992 March/April using receiver B2 and the AOSC backend at the JCMT as part of a 330–360 GHz spectral line survey of the molecular cloud associated with G34.3+0.15. The spectra were taken in double-sideband mode but were separated for identification by using a frequency offset of 10 MHz. The AOSC has 2048 channels with 0.25-MHz spacing and a frequency resolution of 0.33 MHz. The centre frequencies of the upper and lower sidebands are separated by 7.88 GHz. The JCMT has, at 345 GHz, a half-power beamwidth $\theta_{HPBW} = 14$ arcsec, a beam efficiency of 0.55 and a forward-scatter coefficient of $\eta_{fss} = 0.75$. The total system noise was typically less than 1500 K and the data were calibrated using the standard hot/cold-load chopper wheel technique to give line brightness T_A^*. A standard Gaussian-fitting routine was used to determine line parameters and the sideband ambiguity was resolved by comparison with the 10-MHz-shifted spectrum. A list of more than 350 lines, to a detection limit of $T_A^* = 0.3$ K, was compiled over the 30-GHz range, a line density about twice that seen in Orion-KL to a detection limit of 1 K (Jewell et al. 1989), or Sgr B2 (Sutton et al. 1991) and IRC+10216 (Avery et al. 1992) to the 0.3-K level.
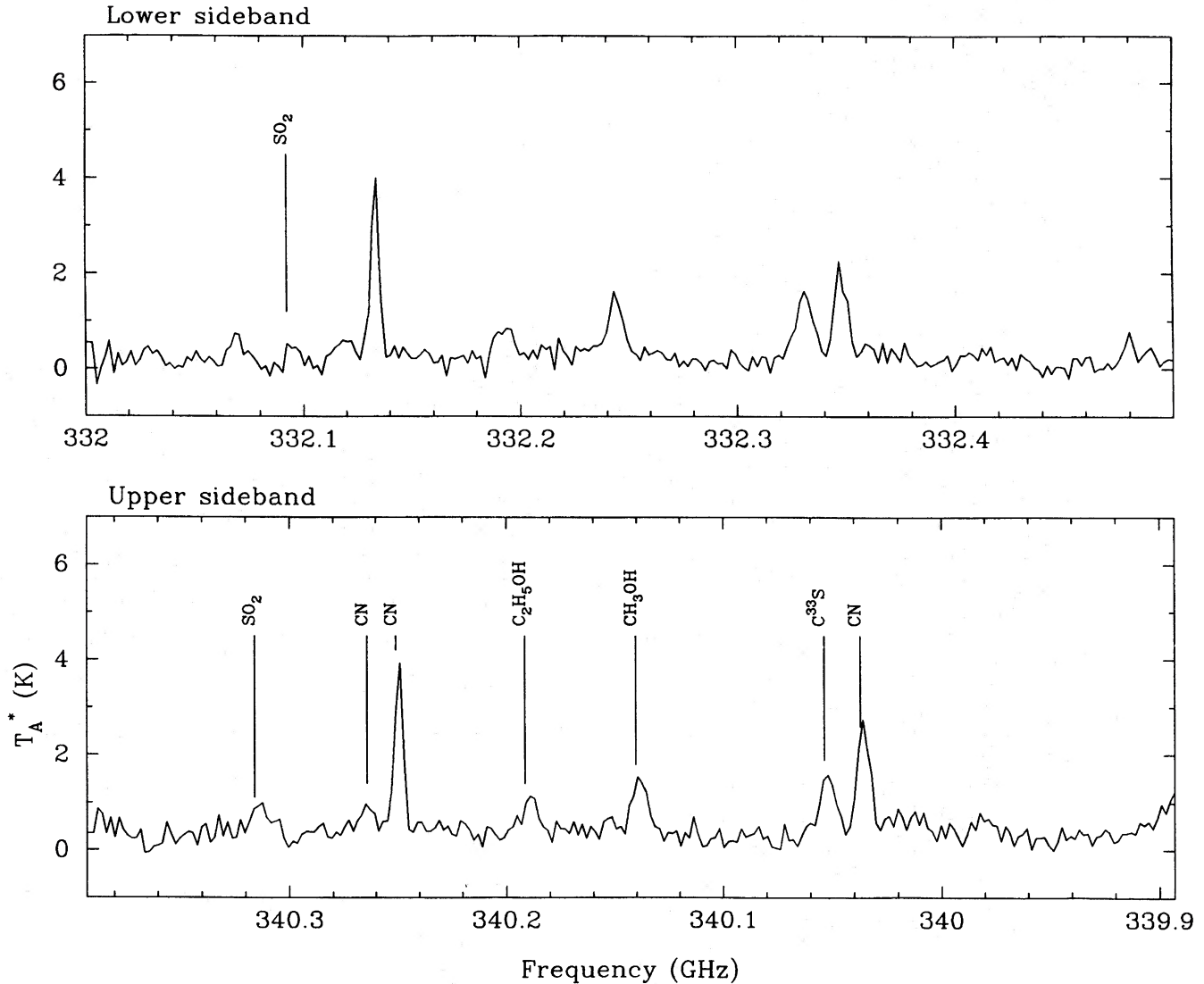
Figure 1. Double-sideband spectra including the $6_{5,2}-5_{4,1}$ and $6_{5,1}-5_{4,2}$ lines of ethanol at 340 189 MHz. Frequency scales shown correspond to lower sideband (top) and upper sideband (bottom) components. The local oscillator frequency for the lower spectrum was increased by 10 MHz for sideband identification. A velocity of 58 km s^{-1} relative to the local standard of rest has been assumed.

Identifications were made with reference to several catalogues: SLAIM, the Jewell et al. (1989) list of Orion-KL detections, the microfiche database of Poynter & Pickett (1984), and transitions tabulated for methanol, CH_3OH, and its isotopic variants by Anderson, Herbst & De Lucia (1987, 1990a,b, 1992, 1993), methyl formate, $HCOOCH_3$, by Plummer et al. (1984, 1986, 1987) and dimethyl ether, CH_3OCH_3, by Herbst (private communication), amongst others. Comparison with a new list of ethanol frequencies based on laboratory and theoretical work by Pearson et al. (1995) revealed eleven coincidences with unidentified (U) lines and three further coincidences with two features previously identified with H_2CCO and CH_3OD. In these cases, the ethanol identification is preferred since many other lines from these species should have been observed.

Additionally, two further U-lines were coincident with very high energy level transitions ($E_u/k > 450$ K) of ethanol at 350 850 and 351 215 MHz but these were rejected since a comparison line of similar energy at 350 960 MHz was not seen. A further U-line at 358 990 MHz is close to an a-type

transition ($S\mu_a^2 = 0.0001$) but was rejected as the only a-type coincidence.

Table 1 lists the 14 transitions identified with the 10 observed features. All are b-type transitions with $S\mu_b^2 > 8.5$ and $E_u/k < 300$ K. A similar search for coincidences between U-lines and several hundred known transitions of ethyl cyanide, CH_3CH_2CN (Pearson et al. 1994), showed no convincing agreements, increasing the significance of the ethanol identifications.

Fig. 1 shows the spectra containing the 340 189-MHz ethanol line, the lower panel with a frequency offset of 10 MHz for sideband identification. The effects of blending with lines in the image band are evident. Other prominent lines are identified as shown: lower sideband lines in the upper panel and upper sideband lines in the lower panel.

3 COLUMN DENSITY ESTIMATE

We have used the data in Table 1 to construct a rotation diagram for ethanol, Fig. 2. The rotation diagram
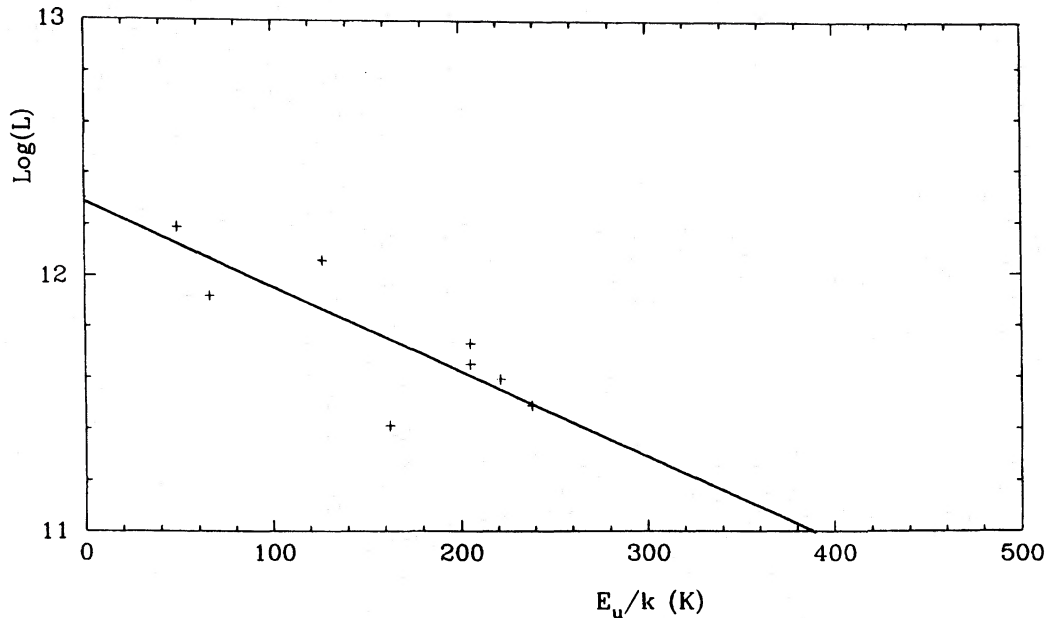
Figure 2. Rotation diagram for ethanol. From this we deduce $T_{rot} = 125$ K and $N = 2.0 \times 10^{15}$ cm^{-2}.

Table 1. Ethanol lines detected in the 330–360 GHz spectrum of G34.3+0.15.

Freq. (MHz)	Transition	$S\mu^2$	E_u (cm^{-1})	T_A^* (K)	Δv (km s^{-1})	Notes
337323	$20_{7,14}$-$20_{6,15}$	20.51	165.4	0.4	5.6	
337727	$19_{7,12}$-$19_{6,13}$	19.19	153.7	0.4	6.7	
338099	$18_{7,11}$-$18_{6,12}$	17.87	142.6	0.5	6.8	
338110	$18_{7,12}$-$18_{6,13}$	17.87	142.6	0.5	5.7	
338886	$15_{7,8}$-$15_{6,9}$	13.90	112.8	0.4	6.4	blend
338887	$15_{7,9}$-$15_{6,10}$	13.90	112.8	0.4	6.4	blend
339313	$12_{7,5}$-$12_{6,6}$	9.82	88.3	0.9	9.0	blend
339313	$12_{7,6}$-$12_{6,7}$	9.82	88.3	0.9	9.0	blend
340189	$6_{5,2}$-$5_{4,1}$	9.39	34.1	0.9	11.7	blend
340189	$6_{5,1}$-$5_{4,2}$	9.39	34.1	0.9	11.7	blend
351918	$25_{3,22}$-$24_{4,21}$	12.08	201.5	0.3	8.2	
357067	$10_{4,7}$-$9_{3,6}$	8.79	46.1	0.5	7.6	
357681	$7_{5,3}$-$6_{4,2}$	9.59	38.1	0.6	7.9	blend
357682	$7_{5,2}$-$6_{4,3}$	9.59	38.1	0.6	7.9	blend

method has been discussed by, among others, Blake et al. (1987) and Turner (1991). Essentially, for emission that is optically thin and characterized by a single excitation temperature T_{rot}, a plot of $\log_{10} L$ versus E_u/k, where $L = 3k \int T_R dv / 8\pi^3 v S\mu^2$, $\int T_R dv$ is the integrated line intensity, v the transition frequency, S the line strength, μ the permanent electric dipole moment, and E_u the energy of the upper level, gives a straight line of slope $-\log_{10} e/T_{rot}$ and intercept $\log_{10}[g_K g_I N/Q(T_{rot})]$, where the product of the degeneracies $g_K g_I = 2$ for all ethanol transitions observed here, N is the total column density and $Q(T_{rot})$ is the rotational partition function.

The observed T_A^* for the three pairs of blended lines at 338 886, 339 313 and 340 189 MHz is assumed to have an equal contribution from each of the two components. Data for the blended pair of lines at 357 681 MHz were not used

due to severe confusion with broad SO_2 lines at 357 672 MHz. Similarly, the weakest line detected, at 351 920 MHz, was neglected due to confusion. From the remaining 11 data points (5 singles + 3 pairs) we derive a best-fitting rotational temperature of 125_{-25}^{+45} K and a column density, averaged over the 14-arcsec beam, of $1.9_{-0.7}^{+1.1} \times 10^{15}$ cm^{-2}. If, as appears likely, ethanol arises in the compact hot core of G34.3+0.15, which has a source size of about 4 arcsec as derived from interferometric maps of CH_3CN (Macdonald & Habing 1994), then $N = 2.4_{-0.9}^{+1.2} \times 10^{16}$ cm^{-2}. The large rotation temperature of 125 K is consistent with, although somewhat smaller than, the 320-K dust temperature observed by Hauschildt, Güsten & Schilke (1994), the 230-K gas kinetic temperature derived from H_2CO observations by Magnum & Wootten (1993) and the 240–275 K NH_3 kinetic temperature derived by Garay & Rodriguez (1990). In addition, Macdonald & Habing (1994) derive $T = 200$–315 K from CH_3CN measurements, with some evidence that the higher J lines probe hotter and denser gas within the core. Our derived rotational temperature may be regarded as a lower limit since the highest level used in our analysis has an energy, E_u/k, of 238 K and, in addition, it is possible that, if strong temperature gradients exist in the core, the higher transitions are more beam-diluted than the lower.

We have, as part of the spectral scan, detected many lines of methyl formate, $HCOOCH_3$, and some weak lines of dimethyl ether, CH_3OCH_3. We have enough unblended lines to derive the column density and rotation temperature of methyl formate, but not those of dimethyl ether. For methyl formate, we find $N = 9.8 \times 10^{15}$ cm^{-2} and $T_{rot} = 52$ K. The total column density of H_2 is difficult to estimate in G34.3+0.15, as indeed it is in all hot cores, but, based on observations of HCO^+ and the dust continuum at 450 μm (Heaton et al. 1993; Strong-Jones, Heaton & Little 1989), $n(H_2) = 8.8 \times 10^5$ cm^{-2} within a radius of 0.1 pc (7 arcsec). Thus, over our 14-arcsec beam, $N(H_2) = 5.3 \times 10^{23}$ cm^{-2}, giving a fractional abundance for ethanol of 4×10^{-9}, and for methyl formate of 2×10^{-8}. For

a source size of 4 arcsec and $n(H_2) = 10^7$ cm^{-3} (Macdonald & Habing 1994), the fractional abundance of ethanol is 1.5×10^{-8}.
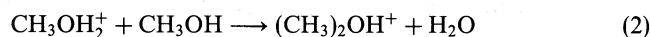
4 DISCUSSION

The ultra-compact H II region associated with G34.3+0.15 has a classical cometary shape believed to be due to a bow shock caused by the impact of the stellar wind and the ambient cloud. This shock and its associated heating both release mantle material from cold interstellar grains and chemically process the gas. VLA observations of NH$_3$ (Heaton, Little & Bishop 1989) show that the molecular cloud is wrapped around the head of the H II region. Recent JCMT and Nobeyama Millimetre Array observations of CH$_3$CCH and CH$_3$CN by Macdonald & Habing (1994) have shown that there is an offset in both position and velocity between CH$_3$CN and NH$_3$ which is consistent with a scenario in which ammonia is evaporated from the grains, swept parallel to the bow shock and processed into methyl cyanide on a time-scale of $\approx 10^5$ yr.

Charnley, Tielens & Millar (1992) have investigated the detailed formation of complex molecules upon the evaporation of simple hydrides in hot core sources. Although a number of such species can be formed rapidly, the models, which were developed specifically for the hot cores in Orion, do not account for the observed abundance of ethanol, even when methanol is evaporated from the grains (Millar, Herbst & Charnley 1991), although as mentioned above the exact column density is uncertain by a large factor. Turner (1991) argues, taking opacity effects into consideration, that $N = (3-8) \times 10^{18}$ cm^{-2}, whereas Johansson et al. (1984) and Blake et al. (1987) find upper limits of 1.3×10^{15} and 7.0×10^{14} cm^{-2}, respectively. On the other hand, Ohishi (private communication) reports $N = 10^{15}$ cm^{-2} and a fractional abundance of $\approx 3 \times 10^{-9}$. Although Ohishi's line parameters are consistent with the presence of ethanol in the Compact Ridge, the spatial distribution is more consistent with an origin in the Hot Core. We have used our derived excitation temperature and column density to calculate the integrated intensities expected for the a-type transitions in the 330–360 GHz range. The strongest transitions have $\int T_A^* dv = 0.007$ K km s^{-1}, compared to our typical 3σ upper limit of 0.024 K km s^{-1}. This indicates that the column density of ethanol is certainly less than 6×10^{15} cm^{-2}, otherwise we would have detected several a-type transitions, and offers no support, at least in this source, for Turner's contention that the ethanol column densities are much larger than those inferred from the b-type transitions alone.

Millar et al. (1991) have argued that complex molecule formation in hot cores is driven by the large amounts of methanol evaporated from grain mantles. This methanol, once protonated in the hot gas, can react with other species, for example, H$_2$CO:

$$CH_3OH_2^+ + H_2CO \longrightarrow H_2COOCH_3^+ + H_2 \tag{1}$$

and CH$_3$OH:

$$CH_3OH_2^+ + CH_3OH \longrightarrow (CH_3)_2OH^+ + H_2O \tag{2}$$

which recombine to form methyl formate, HCOOCH$_3$, and dimethyl ether, (CH$_3$)$_2$O, respectively. However, the injection of methanol does not lead to the formation of ethanol. Instead, as discussed by Millar et al. (1991) and by Charnley et al.

(1992), protonated ethanol is thought to form in the radiative association reaction

$$H_3O^+ + C_2H_4 \longrightarrow C_2H_5OH_2^+ + h\nu \tag{3}$$
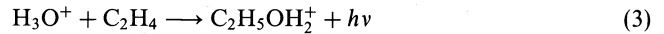
followed by dissociative recombination. Over the temperature range 50–100 K, the rate coefficient, k_3, is estimated to be $1.3 \times 10^{-14} (T/300)^{-3}$ cm^3 s^{-1} (Millar et al. 1991). The steep temperature dependence ensures that this mechanism is inefficient at the temperatures of typical hot cores. Detailed time-dependent models of the chemistry based on the release of methanol from the grains lead to ethanol fractional abundances $\approx 10^{-11}$ (Charnley et al. 1992), far below the abundance reported by Ohishi and even further below the abundance we derive for the hot gas in G34.3+0.15.

Since the observed abundance of ethanol cannot arise in gas-phase reactions, it appears that the ethanol is synthesized on the grain surface before release into the gas phase. Such a conclusion was reached also for methanol (Millar et al. 1991), and suggests that alcohols might be a natural by-product of the grain surface chemistry in star-forming regions. The detailed route by which these species form is, as yet, unclear. The formation of ethanol was discussed by Millar et al. (1988) and, in more general terms, the formation of alcohols on grains has been discussed by Charnley et al. (1995) who favour diffusion-controlled reactions in bulk molecular ices, although H and O atom reactions, driven by quantum tunnelling, with hydrocarbons are also a possibility. Charnley et al. have discussed the chemistry subsequent to the evaporation of the alcohols methanol, ethanol, propanol and butanol. Charnley et al. (1992, 1995) have shown that an injected fractional abundance of 10^{-6} for methanol gives rise to a peak fractional abundance for methyl formate of 10^{-8} after 10^4 yr. Any ethanol injected is destroyed in gas-phase reactions, particularly in dissociative proton transfer with H$_3^+$ (Smith, Spanel & Millar 1994), on a time-scale of about 2×10^4 yr. The ethanol also reacts to produce methyl ethyl ether (CH$_3$OC$_2$H$_5$) and diethyl ether (C$_2$H$_5$OC$_2$H$_5$), with the former likely to be detectable once line frequencies are known. In addition, once the hot gas-phase chemistry of ethanol becomes better known, in particular its reaction rate coefficients with O, OH and O$_2$, it may be possible to use it as a chemical clock in hot core sources.

5 CONCLUSIONS

We have identified 10 emission features in the 330–360 GHz spectrum of the molecular cloud associated with the ultra-compact H II region G34.3+0.15 with 14 rotational lines of ethanol. This appears to be the first unambiguous detection of ethanol in hot gas. Using the rotation diagram method, we find the column density and excitation temperature, averaged over our 14-arcsec beam, to be 2.0×10^{15} cm^{-2} and 125 K, respectively. This column density is large and implies a fractional abundance, with respect to H$_2$, of 10^{-8} for a 4-arcsec source size. This abundance is orders of magnitude larger than can be produced by gas-phase chemistry using known reaction pathways, and implies that the ethanol is the product of grain surface chemistry. Since it has been concluded previously that methanol is produced by grain chemistry, it appears that alcohols may be a natural by-product of surface chemistry in interstellar clouds.

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