

## On the source of cometary $\text{N}_2^+$ ions

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**Abstract.** The possibility of nitrous oxide ( $\text{N}_2\text{O}$ ) molecules in Comet 1P/Halley (Saxena 2004) is revisited in the light of theoretical considerations, its detection in hot molecular cores and observations of annealed Mg-silicate grains in comets to support its parent nature in other comets as well. Having a photolifetime  $\geq 10^5$ s at 1 AU heliocentric distance (Huebner et al. 1992),  $\text{N}_2\text{O}$  may be the source of  $\text{N}_2^+$  ions in cometary tails. The detection of  $\text{N}_2\text{O}$  molecule in comets will have important implications on the nature of cometary parent molecules.

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### 1. Introduction

Molecular nitrogen ion ( $\text{N}_2^+$ ) can only originate from molecular nitrogen that has never been observed in any astronomical object. In interstellar clouds, it is inferred indirectly from modelling coupled with observations of  $\text{N}_2\text{H}^+$  ion. As all the resonance lines of  $\text{N}_2$  molecules are of wavelengths shorter than Ly- $\alpha$  (A'Hearn & Festou 1990), in comets it is inferred from spectroscopic observations of  $\text{N}_2^+$  ion in the visible region of the spectrum. If  $\text{N}_2^+$  ions are produced from solar ionization of  $\text{N}_2$  molecules sublimating from the cometary nucleus, they should have been detected spectroscopically in the cometary coma itself. Therefore,  $\text{N}_2^+$  ions are unlikely to be produced from  $\text{N}_2$  molecules in comets. The  $\text{N}_2$  molecule is extremely volatile (sublimation temperature  $\sim 20$  K) and is a non-polar molecule that is expected to diffuse easily from the cometary nucleus. In contrast  $\text{N}_2\text{O}$  is a polar molecule having a dipole moment = 0.2D which is comparable to that of CO (dipole moment = 0.1D) and is expected to be entrapped more effectively than  $\text{N}_2$  in  $\text{H}_2\text{O}$  - ice of cometary nucleus.

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In the present work, the possibility of nitrous oxide ( $\text{N}_2\text{O}$ ) as a parent molecule in comet 1P/Halley (Saxena 2004) has been extended to other comets in light of dynamics of the Solar nebula and resemblance of  $10\ \mu\text{m}$  feature of annealed Mg-silicate smoke to the same feature of dust in comets.

## 2. Origin of nitrous oxide ( $\text{N}_2\text{O}$ )

There exists evidence of moderately high temperatures  $\approx 1000\ \text{K}$  prevailing in the innermost Solar nebula sometime during its lifetime and of large scale circular motions capable of transporting dust and gas from this region to distances beyond the snow line (Hugh et al. 2001). These conclusions are based, among other evidences, on almost identical resemblance of the  $10\ \mu\text{m}$  IR feature of Mg-silicate smoke annealed to about  $1000\ \text{K}$  in the laboratory to the same feature of dust observed in Comet 1P/Halley, comet C/1995 OI (Hale-Bopp), Comet Bradfield and Comet Mueller (Hallenbeck et al. 1998).

Oxygen is thermodynamically more stable when it reacts with hydrogen to form water in an oxygen rich environment ( $\text{O} > \text{C}$ ). In an oxygen poor environment ( $\text{O} < \text{C}$ ), oxygen is tied up in CO. However, oxygen is tied up to nitrogen in three observed interstellar N-O bond molecules viz., NO,  $\text{N}_2\text{O}$  and HNO. Their production is, therefore, to be considered in the framework of gas phase ion-molecule and radical-radical reactions. In the inner Solar nebula the gas kinetic temperatures were sufficient to overcome the activation energy barrier of  $19\ \text{meV}$  ( $\cong 210\ \text{K}$ ) of the ion-molecule reaction between  $\text{N}^+$  ion and  $\text{H}_2$  molecule to produce  $\text{NH}^+$  ion (Table 1). This reaction has initially been discussed for the production of ammonia ( $\text{NH}_3$ ) in interstellar clouds. The  $\text{N}^+$  ion results from direct ionization of N atom by cosmic rays and/or from the dissociative ionization of  $\text{N}_2$  molecule by  $\text{He}^+$  ion. Once  $\text{NH}^+$  ion is produced, all other nitrogen hydride ions are produced unhindered. The dissociative electron recombination of the nitrogen hydride ions produces nitrogen hydride radicals and ammonia. The destruction of ammonia through cosmic ray generated  $\text{He}^+$  and  $\text{H}_3^+$  ions also leads to the production of nitrogen hydrides. The nitrogen hydrides in turn produce  $\text{N}_2\text{O}$  molecules from radical-radical reactions (Table 1).

According to the current hypothesis of circular motions in the Solar nebula, transporting material from its innermost part to regions beyond the snow-line (Hugh et al. 2001), the nitrous oxide ( $\text{N}_2\text{O}$ ) produced in the central part of the nebula will likewise be transported along with the dust to the region beyond the snow-line in the nebula. In this region, the  $\text{N}_2\text{O}$  molecules like other volatiles are frozen on to the dust grains in the process of formation of cometesimals.

## 3. Expected abundance of $\text{N}_2\text{O}$ in comets

The value of  $Q(\text{N}_2)/Q(\text{H}_2\text{O}) = 2 \times 10^{-4}$  in the tail of 1P/Halley (Wyckoff et al. 1991; Wyckoff & Theobald 1989) probably is an over estimation of the ratio as the same is

derived from the low resolution spectra and modelling of the weak emission feature in the spectral region 3855 Å - 3950 Å that is a mixture of contributions from  $CO^+$ ,  $CO_2^+$  and  $N_2^+$  ions. The observations of  $N_2^+$  ions in the high resolution spectra of recent comets 122P/1995 S1 (de Vico), C/1995 O1 (Hale-Bopp) and C/2002 C1 (Ikeya-Zhang) have resulted only in upper limits of the ratio  $N_2^+/CO^+$  viz.  $\leq 10^{-5}$  -  $10^{-4}$  (Cochran et al. 2000; Cochran 2002). The upper limits are suggestive of extremely low abundance of  $N_2^+$  ions that is inaccessible with the current instrumentation. Due to kinetic inhibition shown by  $N_2$  and  $CO$  molecules, the ratio  $N_2^+/CO^+$  roughly equals the ratio  $N_2/CO$  and that in turn translates to  $N_2/H_2O \leq 10^{-6}$  -  $10^{-5}$  in these comets assuming  $CO/H_2O \sim 0.1$ .

If  $N_2O$  is a parent of  $N_2$  in comets and as  $\tau(N_2O) \sim \tau(N_2)$ , these upper limits would translate to  $N_2O/H_2O \leq 10^{-6}$ - $10^{-5}$  in these comets. Since the fractional abundance of  $H_2O$  relative to  $H_2$  is on the order of  $10^{-4}$  in comets, we get  $N_2O/H_2 \leq 10^{-10}$  - $10^{-9}$ , which is in fair agreement with the observed fractional abundance  $\sim 10^{-9}$  of  $N_2O$  relative to  $H_2$  in hot molecular cores Sgr B2 (M) and Sgr B2 (N) embedded in Sgr B2 cloud complex. (Zuirys et al. 1994; Halfen et al. 2001).

#### 4. Discussion

In the scenario presented by the possible detection of annealed Mg-silicate dust in several comets, one can visualize a transportation mechanism operative from the central region of higher temperatures in the Solar nebula, the birth place of Mg-silicate dust, to regions of lower temperatures (Hugh et al. 2001) where comets are formed. During this journey, the dust grains and possibly other molecules including  $N_2O$  and  $H_2O$  molecules pass through the region  $\sim 5$ -6 AU from the centre of the nebula where the temperatures are  $\cong 100$ K. The laboratory studies show that at these temperatures the  $H_2O$ -ice is produced in amorphous form (Laufer et al. 1987). Due to the formation of hydrogen bonds, the polar gaseous molecule  $N_2O$  gets trapped in the cometary amorphous ice.

Nitrous oxide ( $N_2O$ ) has been observed as an interstellar molecule in the hot cores of molecular clouds (Zuirys et al. 1994; Halfen et al. 2001). High temperature ( $\sim 200$ - $300$ K) chemistry is involved in the production of  $N_2O$  molecule as is evidenced in Sgr B2 cloud complex where  $N_2O$  is observed as confined exclusively to a region  $\leq 45''$  centered on hot molecular core Sgr B2 (N) and where nearly identical distribution is found for the high energy ( $E_a \approx 225$ K)  $14_0-14_{-1}$  E transition of  $CH_3OH$  (Halfen et al. 2001). Moreover,  $NH_3$  has an abnormally high column density  $\approx 10^{20}$   $cm^{-2}$  in Sgr B2(N). (Ohishi 1997) suggests that  $N_2O$  and  $NH_3$  may be related. Indeed gas phase production of ammonia and also its destruction via cosmic-ray generated reactive ions viz.  $H_3^+$  and  $He^+$  both lead to the production of nitrogen hydrides  $NH$  and  $NH_2$ , the former produces  $N_2O$  from the neutral-neutral reaction:  $NH + NO \rightarrow N_2O + H$  (Halfen et al. 2001). The other hydride viz.  $NH_2$  may also produce  $N_2O$  from the reactions (R18) and (R20) that need no activation energy (Table 1). First discussed in cometary context  $N_2O$  (Saxena 2004) has a photolifetime of  $\geq 10^5$  s at 1AU heliocentric distance (Huebner et al. 1992). With

**Table 1.** Main reactions showing the production of nitrogen hydrides and N<sub>2</sub>O molecule in solar nebula.

Reaction No.	Reaction	Rate coefficient (cm <sup>3</sup> s <sup>-1</sup> )	Ref.
(R1)	$N + CR \rightarrow N^+ + e + CR$	$\zeta$	(1)
(R2)	$He^+ + N_2 \rightarrow N^+ + N + He$	8.10(-10)	(2)
(R3)	$N^+ + H_2 \rightarrow NH^+ + H$	4.80(-10)	(3)
(R4)	$NH^+ + H_2 \rightarrow NH_2^+ + H$		
(R5)	$NH_2^+ + H_2 \rightarrow NH_3^+ + H$	2.70 (-10)	(4)
(R6)	$NH_3^+ + H_2 \rightarrow NH_4^+ + H$	2.00 (-12)	(4)
(R7)	$NH_3^+ + H_2O \rightarrow NH_4^+ + OH$	1.10 (-10)	(4)
(R8)	$NH_4^+ + e \rightarrow NH_3 + H$	$6.80(-7)(T/300)^{-0.6}$	(4)
(R9)	$\rightarrow NH_2 + H_2$	$6.80 (-7)(T/300)^{-0.6}$	(4)
(R10)	$NH_3 + H_3^+ \rightarrow NH_4^+ + H_2$	2.70 (-9)	(4)
(R11)	$NH_3 + He^+ \rightarrow NH_3^+ + He$	2.64 (-10)	(4)
(R12)	$NH_3^+ + e \rightarrow NH_2 + H$	$3.00 (-7)(T/300)^{-0.5}$	(4)
(R13)	$\rightarrow NH + H_2$	$3.00 (-7)(T/300)^{-0.5}$	(4)
(R14)	$NH_2^+ + e \rightarrow NH + H$	$1.50 (-7)(T/300)^{-0.5}$	(4)
(R15)	$NH + O \rightarrow NO + H$	1.16 (-10)	(5)
(R16)	$NH + OH \rightarrow NO + H_2$	3.98 (-11)	(5)
(R17)	$NH_2 + O \rightarrow NO + H_2$	8.30 (-12)	(5)
(R18)	$NH_2 + NO \rightarrow N_2H + OH$	6.59 (-13)	(5)
(R19)	$NH + NO \rightarrow N_2O + H$	$(1-3) \times 10 (-11)$ $125K < T < 300K$	(6)
(R20)	$N_2H + O \rightarrow N_2O + H$	1.67 (-10)	(5)

Note:  $q(p) = q \times 10^p$ , (1):  $\zeta = 2.7(-17) s^{-1}$  (Greadel et al. 1982), (2): Huntress W.T. 1977 (3): Adams & Smith 1985, (4): Millar et al. 1997, (5): Warnatz et al. 1996 (6): Halfen et al. 2001.

a speed of  $\sim 1 km s^{-1}$ , it could reach beyond the cometary coma into the tail of a comet where solar photodissociation followed by solar ionization and/or charge exchange with solar wind  $\alpha$ -particles produce  $N_2^+$  ions.

Nitrous oxide in cometary context assumes importance as its positive detection, besides being consistent with the current hypothesis of the Solar nebula, may be used as a diagnostic for chemically processed molecules residing in the cometary nucleus. The other N-O bond molecule viz. NO has been reported in Comet 1P/Halley (Geiss et al. 1991)

This in turn will have important implications on the nature of cometary parent molecules that are generally believed to be formed only from gas - grain surface chemistry.

## 5. Conclusions

The arguments presented here and elsewhere (Saxena 2004) for  $N_2O$  instead of  $N_2$  as a cometary parent molecule that is responsible for cometary  $N_2^+$  ions are consistent with theory and observations on comets. The detection of  $N_2O$  molecules in future comets is of utmost importance as it will also have implications on the nature of cometary parent molecules.

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