EXCITATION PROCESSES IN COMETARY COMAE

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ABSTRACT:- Excitations of cometary NH and S_2 molecules are discussed. Photodissociation and dissociative electron recombination processes may be sources of meta-stable nitrogen ($^2P^o$, $^2D^o$) atoms in comets.

I.Introduction:- The nucleus of a comet is beleived to contain frozen volatile chemical compounds which are evaporated and are then decomposed by solar radiation field when a comet approaches (or recedes) the sun (Whipple, 1950). The decomposed material surrounds the nucleus and develops an expanding atmosphere of gas and dust which is referred as the coma of a comet and contains dust (possibly ice-coated grains),molecules, neutral radicals, atomic species and molecular ions that are released from the nucleus with velocities of about 0.5-1 km s^{-1}.Over the past centuary a considerable amount of information has been obtained about the composition of coma through spectral line studies extending from ultraviolet (uv) to radiowave (rw) region (see Wyckoff,1982).

II.Excitation of NH:- The NH radical is known to exist in cometary comae (Swings and Haser, 1956),through identification of (0,0) transition of NH($A^3\pi$ - $X^3\Sigma$) at 3360 Å. Recent calculation by Litvak and Kuiper(1982) shows that the resonance fluorescence mechanism is operative for 3360 Å band of the NH radical in comets.Lifetime measurements of NH by high frequency deflection technique (Smith et al. 1976) show that v' = 2 level of NH $A^3\pi$ state undergoes in a predissociation process via spin-orbit coupling ($A^3\pi$, $^5\Sigma$) similar to that of OH. At sun-comet distance = 1 AU, the lifetime of cometary NH radical varies from 1.3 10^4s to 2.3 10^4s for a comet of radial velocity ranging from -80 km s^{-1} to +80 km s^{-1}. Photodissociation of NH by absorption of solar photons through v'=2 level of NH $A^3\pi$ state leads NI($^4S^o$) and HI(^2S) atoms with corresponding velocity of 1 km s^{-1} and 15 km s^{-1}. Photodissociation of cometary NH_3 (Altenhoff et al. 1983) may result NH radical in a process as described by Jackson (1976). At r = 1 AU, total photodissociation lifetime of amonia is about 5.65 10^3 s (Huebner and Carpenter, 1979). If an outstream velocity of NH parent is assumed to be of the order of 1 km s^{-1} then Combi's diaphragm convolution model NH parent scale length,scaled at r = 1 AU, would be of about 5.4 10^3 km (Combi, 1978).

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III. Excitation of NI:-Dissociative electron recombination process of N_2^+ with electron may be a source of NI($^2P^o$, $^2D^o$) atoms in cometary comae (Queffelec et al. 1985). In addition, photodissociation of CN by absorption of solar photons may also result meta-stable nitrogen atoms(Lavendy et al. 1984).The radiative lifetimes of NI($^2P^o$) and NI($^2D^o$) states are about 5.39 s and 3.64 10^4s,respectively (zeippen,1982). At r = 1 AU, the photoionization rates by solar ultraviolet photons for NI($^4S^o$), NI($^2D^o$) and NI($^2P^o$) states are 1.85 10^{-7}, 1.65 10^{-7} and 1.96 10^{-7} s^{-1},respectively. The g-factors, at r = 1 AU, for NI(^4P - $^4S^o$), NI(^2P - $^2D^o$) and NI(^2P-$^2P^o$) transitions, which occur at 1200, 1493 and 1743 A, are 1.1 10^{-5},1.9 10^{-6} and 6.9 10^{-6} s^{-1} ,respectively.The 1200 Å line would be masked by strong Lyman alpha emission of H-atom. If g = $g_e r^{-2}$($g_e$is the g-factor at r = 1 AU) the line NI(^2P - $^2D^o$) at 1493 Å would be excitable by resonance-fluorescence mechanism and may be seen in comets when r is less than o.25 AU. The weak line at 5201.1 Å observed in the spectra of several comets (Swings and Haser, 1956) could be due to forbidden NI($^2D^o$-$^4S^o$) transition (Cosmovici and Ortolani, 1980). The theoretical estimate of intensity ratio NI($^2P^o$-$^2D^o$)/ NI($^2D^o$- $^4S^o$) is of the order of unity and does not depend on solar cycle. The line 5201.1 Å is too weak for any quantitative analysis.

IV. Excitation of S_2:-Emission bands due to S_2($B^3\Sigma_u^- - X^3\Sigma_g^-$) transition in the range 2829-3058 Å have been observed in the uv spectra of comet IRAS Araki-Alcock (1983d) (A'Hearn et al.1983). The observed intensities are in agreement with the intensities estimated by resonance scattering.An abundance of 3 10^{27} S_2 molecules was derived for comet (1983d) by A'Hearn et al. (1983). Vibrational levels v' $\geq$ 10 of the $B^3\Sigma_u^-$ state predissociate and predissociation efficiency of v' = 10 level is 0.92 (Ricks and Barrow, 1969). At r = 1 AU, absorption of solar uv photons of wavelength ~ 280 nm leads to a dissociation lifetime of about 250 s for S_2 (de Almeida and Singh, 1986) which is a factor of two lower than that used by A'Hearn et al. (1983). Since solar flux at wavelength ~280 nm does not vary much we have neglected the dependence of lifetime of S_2 on heliocentric velocity of comet. A S_2 production rate of about 1.2 10^{25} s^{-1} is derived for comet (1983d) which is comparable to CS production rates derived for comet (1983d) (A'Hearn et al. 1983), Bradfield (Jackson et al. 1982) and Encke (Feldman et al. 1984; Weaver et al. 1981) when the data are compared at about the same heliocentric distance. If $Q(H_2O) \sim 10^{29}$ s^{-1} for comet (1983d), the ratio $Q(S_2)/Q(H_2O) \sim 10^{-4}$. Observed spatial profile of the (7,0) band indicates that S_2 are released very near to the nucleus of the comet (1983d) (A'Hearn et al. 1983). For comet Bradfield, the CS and S production rates follow about the same heliocentric variation ($Q(CS) \propto r^{-5}$ and $Q(S) \propto r^{-5.4}$) and thus indicate a common parent for both species (Jackson et al. 1982). Photodissociation of CS_2 at wavelength of the order of 193 nm (Yang et al. 1980) yields:

$$CS_2 + h\nu \longrightarrow CS(X^1\Sigma^+) + S(^3P) \quad (1)$$

$$CS_2 + h\nu \longrightarrow CS(X^1\Sigma^+) + S(^1D) \quad (2)$$

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CS vibrationally excited to v" = 7 and branching ratio is 20% for (1) and 80% for (2). The radiative lifetime of S(^{1}D) state is about 28 s (Weise et al. 1966) and, analogous to OI, transitions : SI($^1D_2 - {}^3P_1$) and SI($^1D_2 - {}^3P_2$) may be detectable at 11305.8 Å and 10819.8 Å, respectively, in comets. In the inner coma, the reaction:

$$S(^1D) + CS_2 \longrightarrow CS + S_2 \qquad (3)$$

may result S_2 in v" ≤ 8 of the $X^3\Sigma_g^-$ state (Venkitchalam and Krishnamachari, 1980). The excited S_2 molecules will come to the v"=0 level by collision deactivation process. The rate constant of (3) is not known. H_2S is isovalent to H_2O and photodissociation of hydrogen sulphide will result SH which by neutral-radical reaction may yield S_2:

$$H_2S + h\nu\,(193\ nm) \longrightarrow SH + H \qquad (4)$$

$$SH + S \longrightarrow S_2 + H \qquad (5)$$

The dissociation energy of H_2S is about 3.26 eV compared to dissociation energy of water molecule of about 5.1136 eV and photodissociation of H_2S yields a velocity distribution of about 16 km s^{-1} for hydrogen atoms which fits well with high component H-atoms found in comets (Festou et al. 1983). The (0,0) band of SH($A^2\Sigma - X^2\pi$) appears at 3261 Å and would be blended with cometary CO^+_2 emission (Festou et al. 1982). Further, H_2S^+ (ionization potential of H_2S is ~10.472 eV compared to ionization potential of H_2O = 12.618 eV) ion has recently been identified in comet(1983d) by Cosmovici and Ortolani (1984) and Bradfield by Cosmovici et al. (1982). H_2S is known to occur in interstellar sources (Thaddeus and Kutner,1972) and cometary theoretical models (Yamamoto et al. 1983) having interstellar compositions have resulted cometary molecular abundances in agreement with those found in comets. This suggests an indirect evidence of H_2S in the nucleus of a comet. A recent attempt for detection of H_2S at 1.59 micron band in comet West by Johnson et al. (1983) was unsuccessful. If $k_5 \sim 10^{-11}$ cm^3 s^{-1} (typical neutral-radical reaction rate constant - Liszt, 1978, Millar, 1982) the time scale for reaction (5) would be about 28 hours when the density in the inner coma is of the order of 10^6 cm^{-3}.

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DISCUSSION

MITCHELL: It is premature to rule out interstellar S_2 as the source of cometary S_2. The observed interstellar upper limit is not restructure, being $S_2/n \leq 10^{-6}$ (Liszt 1978). An ion-molecule route to S_2 is $S^+ + H_2S \rightarrow S_2H^+ + H$, $S_2H^+ + e \rightarrow S_2 + H$. S_2 is destroyed by C and O. If interstellar C and O are low in abundance or if the activation energy is reaonably high, S_2 abundance should result. The above path to S_2 has yet to be included in kinetic calculations.

P.D. FELDMAN: I like to comment on your scheme as I find it completely in disagreement with the data that I showed the other day. You produce ^1D sulphur from dissociation of CS_2 and SH from dissociation of H_2S. Both of these need certain time while molecules are going to flow out and then you require two-body collision, which is relatively unlikely. Therefore, I find that any H_2S you produce cannot be concentrated so close to the nucleus as we observed.
P.D. SINGH: I agree with you.

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