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Production of sulphur dimers (S_2) in Comet C/1996 B2 (Hyakutake)

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Abstract. The reaction mechanism involving the association of two sulphur atoms through ethylene (C_2H_4), the latter acting as a catalyst to produce cometary sulphur dimers (S_2) (Saxena & Misra, 1995), has been employed to compute their production rate in Comet C/1996 B2 (Hyakutake). The computed production rate $\sim 4.9 \times 10^{24}$ molecules s^{-1} at UT 24.5 March 1996 agrees well with the reported production rates on March 27, 1996, viz., 6.5×10^{24} molecules s^{-1} or 1×10^{25} molecules s^{-1} based on observations for the two reported lifetimes of S_2 molecules (Laffont et al., 1998). The location of S_2 molecules is found to be very near to the cometary nucleus (nucleocentric.distance $\sim$ 1000 km).

Keywords : molecular processes - comets; individual; C/1996 B2 (Hyakutake).

1. Introduction

The $S_2(B^3\Sigma_u^- - X^3\Sigma_g^-)$ transitions in emission in the spectral range λ2850–3050Åwere first observed in the spectra of Comet C/1983 H1 (IRAS-Araki-Alcock), obtained with IUE space-craft when the Comet was closest ($\Delta = 0.032$ au) to the Earth (A'Hearn et al., 1983). Subsequently the UV spectra of comet 1P/Halley also showed the presence of S_2 molecules in its coma. The spectra of other previous comets, when re-examined, revealed that S_2 is a common feature of cometary spectra (Krishnaswamy & Wallis, 1987).

The cometary S_2 molecules are generally believed to be of parent nature (A'Hearn et al., 1983; A'Hearn and Feldman, 1985; Grim and Greenberg, 1987; Feldman, 1987; A'Hearn, 1992). Putting forward the arguments against the parent nature of S_2 molecules, we proposed a reaction

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mechanism involving the association of two sulphur atoms through ethylene, the latter acting as a catalyst as an alternative for the production of cometary S_2 molecules in Comet 1P/Halley (Saxena & Misra, 1995) which could also account for its observed production rate and location very near to the cometary nucleus.

The presence of S_2 molecules has also been reported in Comet C/1996 B2 (Hyakutake). The reported presence of ethane (C_2H_6) which could dissociate into ethylene (C_2H_4) and a total gas production rate ($\sim$ a few times 10^{29} molecules s^{-1}) relatively similar to Comet IP/Halley, implying similar physical conditions in their comae, provides another opportunity to test the proposed mechanism.

The purpose of the present paper is to examine our proposed reaction mechanism for the production of S_2 molecules in Comet C/1996 B2 (Hyakutake), the coma of which is quite dense, having number densities of $\sim 10^{12}$ to 10^{8} cm^{-3} in the region $\sim$ 1000 kms from the cometary nucleus. In this paper, we theoretically compute the total production rate of S_2 molecules in the coma of Coment C/1996 B2 (Hyakutake) at UT 24.5 March 1996 and compare it with the observed production rate on the nearest date.

2. The adopted model of the innermost coma of Comet C/1996 B2 (Hyakutake)

In present paper we consider the Haser model of the coma of Comet C/1996 B2 (Hyakutake) which assumes isotropic outflow of gas from the nuclear surface with constant velocity. We consider the coma region upto 10^3 km from the nucleus. Model studies show that the velocity of the molecules changes very slowly in the nucleocentric region upto 10^3 km in Comet Halley (Krishna Swamy, 1997). The gas velocity which is based on observations of the coma of Comet C/1996 B2 (Hyakutake) is 0.75 Km s^{-1} (Lis et al., 1997). We have adopted this value of the velocity in the model considered.

Radial symmetry of the parent (neutral) molecules is assumed (Huebner, 1987). The dissociation energies of the sulphur bearing parent molecules considered in the paper viz., H_2S, CS_2 and OCS respectively correspond to solar radiation of wavelengths λ 3160 Å, λ 2792 Å and λ 3973 Å while the wavelength corresponding to the dissociation energy of ethane (C_2H_6), where the product is ethylene (C_2H_4), is λ 8743 Å (Levine, 1985). All of these wavelengths are greater than λ 2424.6 Å which corresponds to the dissociation energy of the most abundant cometary H_2O molecules. The coma of Comet C/1996 B2 (Hyakutake) may, therefore, be treated as optically thin in the present context.

The number density $n_0(X)$ of the molecules of species X at the surface of cometary nucleus is given by

$$n_0(X) = \frac{Q(X)}{4\pi R_N^2 \mathrm{v}(X)} \ \mathrm{cm}^{-3} \tag{1}$$

where, $Q(X)$ is the production rate of molecules $X(s^{-1}), 4\pi R_N^2$ is the surface area of the cometary nucleus of radius R_N (cm^2), $v(X)$ is the expansion speed of molecules X (cm s^{-1}) and X is H_2S and CS_2, OCS. The number density $n_r(X)$ of molecules X at nucleocentric distance r is computed from the relation (Marconi et al., 1990):

$$n_r(X) = \frac{n_0(X)}{r^2} R_N^2 \exp\{-(r - R_N)/v(x)\tau(x)\} \tag{2}$$

where, $\tau(x)$ is the photolifetime of molecules X. Using the production rates/abundances, photolifetimes, and expansion speed from Table 1, the number densities of sulphur bearing parent molecules as computed from equation (1) and (2) are tabulated in Table 2. A radius of 2.4 Km has been adopted for the nucleus of Comet C/1996 B2 (Lisse et al., 1999).

Table 1. Production rates, abundances, photolifetimes and expansion speed of parent molecules in Comet C/1996 B2 (Hyakutake).

Parent Molecule (X)	Production rates $Q(X)$ (Molecules s^{-1})	Abundance N(X)/N (H_2O) (%)	Photo-lifetime (sec.)†	Expansion speed (Km s^{-1})
H_2O	1.9(29)$^{(a)}$		8.20(4)$^{(f)}$	
H_2S		0.6$^{(d)}$	3.95(3)$^{(g)}$	
CS_2		0.1$^{(e)}$	3.50(2)$^{(h)}$	0.75$^{(i)}$
OCS	3.5(26)$^{(b)}$		1.06(4)$^{(i)}$	
C_2H_6	6.4(26)$^{(c)}$		6.05(4)$^{(g)}$	

Note: $q(p) = q \times 10^p$, (a) Dello Russo & DiSanti (1998), (b) Bockelée-Morvan et al., (2000), (c) Mumma et al., (1996), (d) Bockelée-Morvan (1997), (e) Despois et al., (1997), (f) Weaver et al., (1987), (g) derived value, Geiss et al., (1991), (h) Huebner et al., (1992), (i) Crovisier (1994), (j) Lis et al (1997).

†: at 1 au heliocentric distance during solar minimum period. Production rates refer to 1.06 au heliocentric distance while abundances are average values.

3. The reaction mechanism for the sulphur dimers in Comet C/1996 B2 (Hyakutake)

The catalytic reaction mechanism

(R1) $C_2H_4 + S \rightarrow C_2H_4S$; $k_1 = 1.2 \times 10^{-12}$ cm^3 s^{-1} (Phillips & Slater, 1972)

(R2) $C_2H_4S + S \rightarrow C_2H_4 + S_2$; k_2

involving the association of two sulphur atoms through ethylene, the latter acting as a catalyst has been proposed by us (Saxena & Misra, 1995) as an alternative for the production of cometary S_2

Table 2. Number densities (cm^{-3}) of sulphur-bearing parent molecules at various nucleocentric distances in Comet C/1996 B2 (Hyakutake) at 1.06 a.u. heliocentric distance.

Nucleocentric distance (Kms)	[H_2S]	[OCS]	[CS_2]
2.4	4.356(11)	9.215(9)	8.206(11)
5	1.003(11)	2.122(9)	1.874(11)
10	2.503(10)	5.303(8)	4.606(10)
20	6.240(9)	1.324(8)	1.113(10)
30	2.765(9)	5.879(7)	4.782(9)
40	1.550(9)	3.303(7)	2.600(9)
50	9.895(8)	2.111(7)	1.608(9)
100	2.437(8)	5.250(6)	3.394(8)
150	1.067(8)	2.320(6)	1.273(8)
200	5.912(7)	1.297(6)	6.044(7)
250	3.727(7)	8.260(5)	3.265(7)
300	2.550(7)	5.704(5)	1.913(7)
350	1.845(7)	4.167(5)	1.186(7)
400	1.391(7)	3.172(5)	7.667(6)
450	1.083(7)	2.493(5)	5.112(6)
500	8.644(6)	2.008(5)	3.495(6)
550	7.038(6)	1.650(5)	2.437(6)
600	5.825(6)	1.378(5)	1.728(6)
650	4.890(6)	1.168(5)	1.243(6)
700	4.153(6)	1.001(5)	9.047(5)
750	3.564(6)	8.677(4)	6.651(5)
800	3.086(6)	7.584(4)	4.934(5)
850	2.692(6)	6.680(4)	3.688(5)
900	2.366(6)	5.925(4)	2.776(5)
950	2.092(6)	5.288(4)	2.103(5)
1000	1.859(6)	4.746(4)	1.602(5)

Note: $q(p) = q \times 10^p$.

molecules in Comet 1P/Halley. We employ this mechanism for the production of S_2 molecules in Comet C/1996 B2 (Hyakutake).

In the first reaction (R1), the product formed is episulphide. Further reaction of $S(^3P)$ atoms with ethylene episulphide (reaction R(2)) is extremely rapid and forms the basis of a catalysed recombination mechanism for the sulphur atoms to form sulphur dimers (S_2) (Phillips & Slater, 1972).

The suggestion that the above reaction mechanism could be the source of cometary S_2 molecules is based on the considerations already discussed earlier in the case of Comet 1P/Halley (Saxena & Misra, 1995) viz., activation energy consideration and catalytic nature of the reaction mechanism.

4. The OH and C_2H_4 number densities

The OH and C_2H_4 number densities at various nucleocentric distances in Comet C/1996 B2 (Hyakutake) have been computed by assuming the Haser model (1957) which was proposed as a method of modelling the gas distribution in a cometary coma.

Ethane (C_2H_6) has so far been detected in only two comets viz., Comet C/1996 B2 (Hyakutake) and Comet C/1995 01 (Hale-Bopp). C_2H_6 dissociates in a single step to form C_2H_4 (Levine, 1985). The Haser Model assumes that (i) the cometary coma is spherically symmetrical, (ii) the parent-to-daughter process is photolytic, (iii) only one possible parent exists for each daughter, and (iv) the parent dissociates in a single step to form the daughter. The form of the Haser model is

$$n_r(X) = Q(Y)(4\pi r^2 v)^{-1} \frac{(\beta_0)}{\beta_1 - \beta_0}(e^{-\beta_0^r} - e^{-\beta_1^r}) \tag{3}$$

where $n_r(X)$ is the number density of the daughter species $X, Q(Y)$ is the production rate of the parent molecule Y, r is the radial position within the coma, β_0 and β_1 are respectively is the reciprocal scale lengths of the parent species Y and the daughter species X. The scale length ℓ, of a gaseous species is defined as $\ell = \tau v$, where τ and v are respectively the photolifetime and the flow speed of the gaseous species.

Thus, the hydroxyl radical (OH) and the ethylene (C_2H_4) as the daughters and H_2O and C_2H_6 as their respective parents fit well into the criteria i) to iv) given above.

From equation (3), therefore, the number densities $n_r(OH)$ and n_r (C_2H_4) at various nucleocentric distance within the coma of Comet C/1996 B2 (Hyakutake) have been computed at UT 24.5 March, 1996 (heliocentric distance: 1.06 a.u.) using:

$Q(H_2O) = 1.9 \times 10^{29}$ molecules s^{-1} (Dello Russo & DiSanti, 1998)

$\tau\,(H_2O) = 8.2 \times 10^4$ s (Weaver et al., 1987)

$\tau\,(OH) = 1.1 \times 10^5$ s (Gérard, 1990)

$\tau(C_2H_6) = 6.05 \times 10^4$ s (Geiss et al., 1991)

$v(H_2O) = v(OH) = v(C_2H_6) = v\,(C_2H_4) = 0.75$ km s^{-1} (Lis et al., 1998)

$\beta_0\,(H_2O) = 1.44 \times 10^{-5}\,km^{-1}, \beta_0\,(C_2H_6) = 1.96 \times 10^{-5}\,km^{-1}$

$\beta_1\,(OH) = 1.08 \times 10^{-5}\,km^{-1}, \beta_1\,(C_2H_4) = 5.05 \times 10^{-5}\,km^{-1}$

The above photolifetime (τ_s) refer to 1 a.u. heliocentric distance. They have been scaled to 1.06 a.u. heliocentric distance using the relation $\tau \alpha r^2$ (Spinrad, 1987). The number densities of the daughter species OH and C_2H_4, thus derived have been tabulated in Table 3.

Table 3. Number densities (cm^{-3}) of OH and C_2H_4 based on Haser Model at various nucleocentric distances in Comet C/1996 B2 (Hyakutake) at 1.06 a.u. heliocentric distance.

Nucleocentric distance (Kms)	[OH]	[C_2H_4]
2.4	1.216(8)	8.945(5)
5	5.839(7)	4.293(5)
10	2.919(7)	2.146(5)
20	1.459(7)	1.072(5)
30	9.729(6)	7.149(4)
40	7.296(6)	5.360(4)
50	5.836(6)	4.286(4)
100	2.916(6)	2.139(4)
150	1.943(6)	1.424(4)
200	1.456(6)	1.066(4)
250	1.164(6)	8.513(3)
300	9.696(5)	7.082(3)
350	8.306(5)	6.059(3)
400	7.263(5)	5.293(3)
450	6.452(5)	4.696(3)
500	5.803(5)	4.219(3)
550	5.272(5)	3.829(3)
600	4.829(5)	3.504(3)
650	4.455(5)	3.228(3)
700	4.134(5)	2.992(3)
750	3.856(5)	2.788(3)
800	3.613(5)	2.609(3)
850	3.398(5)	2.451(3)
900	3.207(5)	2.311(3)
950	3.036(5)	2.186(3)
1000	2.883(5)	2.073(3)

Note: $q(p) = q \times 10^p$.

5. The atomic sulphur

We consider the observed sulphur bearing parent molecules viz., H_2S, CS_2 and OCS which dissociate under solar radiation field to produce sulphur atoms in the coma of the comet. Therefore photolytic reactions only are of relevance in the present context. Any subsequent two body reaction(s) in the coma resulting in the production of sulphur atom(s) in the cometary coma would be much slower because the rate coefficients of such reactions are many orders of magnitude smaller than those of photolytic reactions and also because of small number density of the radicals involved in such reactions.

The sulphur atoms are therefore, produced from the sulphure bearing parent molecules viz., CS_2, H_2S and OCS, observed in Comet C/1996 B2 (Hyakutake) from the following photolytic reactions:

(R3) $CS_2 + h\nu \rightarrow CS + S$; $k_3 = 2.86(-3)s^{-1}$ (Huebner, 1992)
(R4) (i) $H_2S + h\nu \rightarrow H + HS$; $k_4 = 2.53(-4)s^{-1}$ (Geiss *et al.*, 1991)
(ii) $HS + h\nu \rightarrow H + S$; $k_4' = 6.90(-3)s^{-1}$ (Kim & A'Hearn, 1990)
(R5) $OCS + h\nu \rightarrow CO + S$; $k_5 = 9.4(-5)s^{-1}$ (Crovisier, 1994)

The photolifetimes of HS (145 sec.) and H_2S (3.95×10^2 sec.) at 1 au heliocentric distance have been derived from their respective values of 118 sec. (Kim & A'Hearn, 1990) and 3.2×10^2 sec. (Geiss *et al.*, 1991) at 0.9 au heliocentric distance, using the relation $\tau \alpha r^2$ (Spinrad, 1987). The rate limiting reaction is therefore, the slower one viz., reaction (R4(i)). The rate coefficients of the above photolytic reactions which refere to 1 a.u. heliocentric distances have been scaled to 1.06 a.u. heliocentric distance in the present work.

The production rate Q(S) of atomic sulphur will thus be given by

$$Q(S) = k_3[CS_2] + k_4[H_2S] + k_5[OCS] \tag{4}$$

Similarly, for the loss of sulphur atoms both the number density of the species involved and the rate coefficient of the reaction are to be considered. We consider the main known reactions responsible for the loss of sulphur atoms. Hydroxyl (OH) radical being by far the most abundant diatomic radical in cometary comae, the loss of sulphur atoms would be mainly governed by its reaction with OH since the rate coefficient of the reaction is also quite large compared to those of other neutral reactions. The number density of ionic species in the coma is too small for the ionic reactiona viz., charge transfer and ion-atom interchange reactions to be of any significance in the loss of sulphur atoms. The loss rate L(S) of atomic sulphure will, therefore, be mainly governed by the following reactions:

(R6) $S + OH \rightarrow SO + H$; $k_6 = 1.0(-10)$ cm^3 s^{-1} (Leen & Graff, 1988)
(R7) $S + C_2H_4 \rightarrow C_2H_4S$; $k_7 = 1.2(-12)$ cm^3 s^{-1} (Phillips & Slater, 1972)
(R8) $S + h\nu \rightarrow S^+ + e$; $k_8 = 1.2(-6)s^{-1}$ (Geiss *et al.*, 1991)

The loss rate L(S) of atomic sulphur will be given by

$$L(S) = k_6[OH] + k_7[C_2H_4] + k_8 \tag{5}$$

The number density of S atoms will be given by

$$
\begin{aligned}
[S] &= \frac{\text{production rate Q(S)}}{\text{Loss rate L(S)}} \\
&= \frac{k_3[CS_2] + k_4[H_2S] + k_5[OCS]}{k_6[OH] + k_7[C_2H_4] + k_8} \text{cm}^{-3}
\end{aligned} \tag{6}
$$

Using the number densities of CS_2, H_2S and OCS from Table 2 and the OH and C_2H_4 number densities from Table 3, the production rate, the loss rate and the number density of atomic sulphur at various nucleocentric distances are computed from equations (4), (5) and (6) respectively. The number of sulphur atoms at various nucleocentric distances is shown in Figure 1.

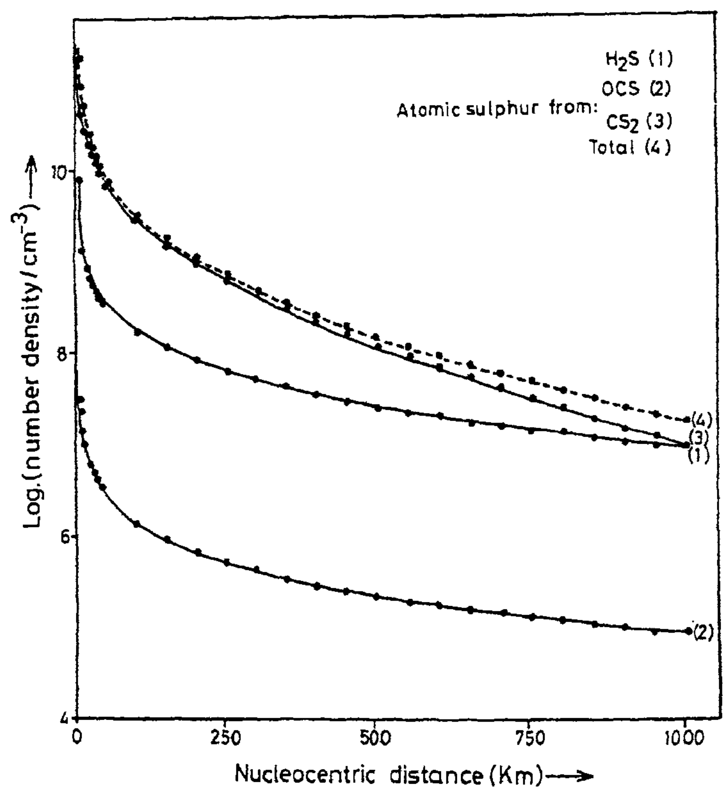

Figure 1. Variation of atomic sulphur as obtained from H_2S, OCS and CS_2 with nucleocentric distance in the coma of Comet C/1996 B2 (Hyakutake).

6. Computation of the production rate of S_2 molecules

As reaction (R2) is extremely rapid and immediately follows reaction (R1), the production rate Q(S_2) of sulphur dimers will be governed by the rate limiting slower reaction (R1), and will therefore be equal to the production rate of ethylene episulphide:

$$Q(S_2) = k_1[C_2H_4][S] \tag{7}$$

The production rate $Q_r(S_2)$ of sulphur dimers at various nucleocentric distances, as computed from equation (7) using the number density of ethylene (C_2H_4) from table 3 and that of atomic sulphur (S) as derived from equation (6) is shown in Figure 2.

To compute the total production rate of S_2 molecules in Comet C/1996 B2 (Hyakutake), the procedure adopted is as follows:

1. The production rates $Q_r(S_2)$ of S_2 molecules are computed at the nuclear surface ($r = 2.4$ km) and at nucleocentric distances $r = 5, 10, 20, 30, 40, 50, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700, 750, 800, 850, 900, 950$ and 1000 km.
2. The nucleocentric region upto 1000 km from the nuclear surface is thus divided into 25 annular shells. The mean of the production rates $Q_r(S_2)$ at the inner and the outer radii of an annular shell, multiplied by its volume, yields the contribution of that shell towards the production rate of S_2 molecules.
3. By summing the respective contributions of each shell, the total production rate of S_2 molecules upto a nucleocentric distance of 1000 km from the cometary nucleus is computed, and is found to be 4.9×10^{24} molecules s^{-1} in Comet C/1996 B2 (Hyakutake) (Figure 3).

7. Discussion

The detection of S_2 molecule in Comet C/1996 B2 (Hyakutake) using HST on April 1, 1996 was reported by Weaver *et al.* (1996). However, with the IUE satellite, its detection on March 27, 1996, five days prior to the HST observations was later reported (Laffont, *et al.*, 1998). The observed production rate $Q(S_2)$ on March 27, 1996 is $Q(\tau_{250s}) = 1 \times 10^{25}$ molecules s^{-1} or $Q(\tau_{450s}) = 6.5 \times 10^{24}$ molecules s^{-1} depending on the lifetime of S_2 molecule (Laffont *et al.*, 1998) which are $\tau_{s_2} = 250s$ (deAlmeida & Singh, 1986) $\tau_{s_2} = 450s$ (A'Hearn *et al*, 1983; Budzien & Feldman, 1992).

We have computed $Q(S_2)$ on the nearest date available viz., UT 24.5 March, 1996 on which observations on $Q(H_2O)$, Q(OCS) and $Q(C_2H_6)$ are reported in literature (Mumma *et al.*, 1996; Dello Russo *et al.*, 1998). For H_2S and CS_2, we have used their reported average abundances at

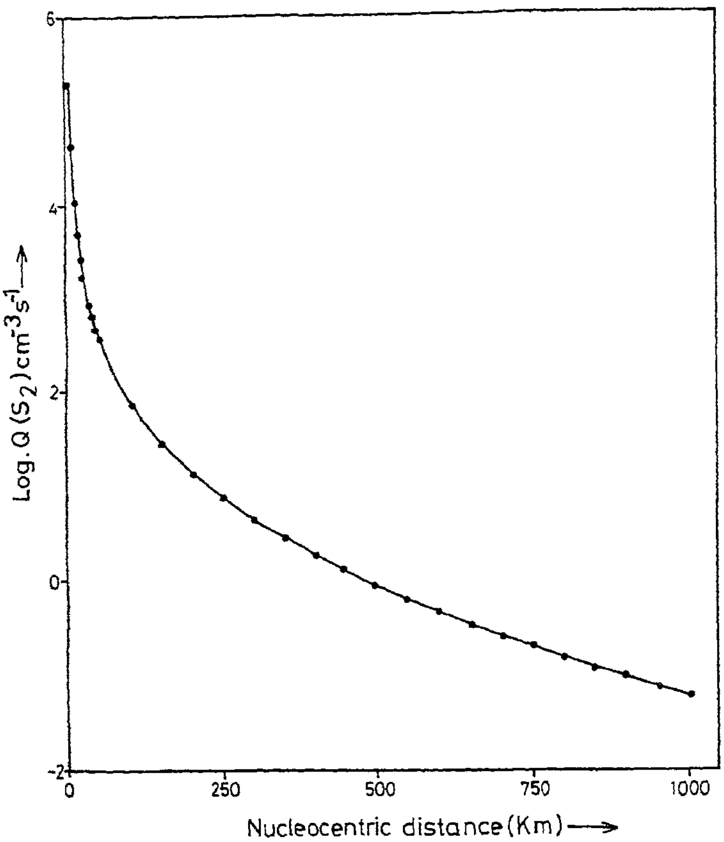

Figure 2. Production rate of S_2 molecules at various nucleocentric distances in Comet C/1996 B2 (Hyakutake).

1 au. heliocentric distance (Bockelée-Morvan, 1997; Despois *et al.*, 1997) in our computations. The $Q(S_2)$ of 4.9×10^{24} molecules s^{-1} on UT 24.5 March, 1996 as computed from the chemical mechanism when the comet was at a heliocentric distance of 1.06 a.u. agrees well with the observed $Q(S_2)$ on March 27, 1996 when the comet was at a heliocentric distance of 0.99 au. The location of S_2 molecules in Comet C/1996 B2 theoretically derived from the chemical mechanism is close to the nucleus (nucleocentric distance $\simeq$ 1000 kms) and is consistent with earlier observations of S_2 molecules (A'Hearn *et al.*, 1983). After Comet IP/Halley, the S_2 molecule was reported in Comet C/1996 B2 (Hyakutake). In both the comets, the proposed chemical mechanism (Saxena & Misra, 1995) could account for the observed production rate of S_2 molecules, despite so many uncertainties regarding (i) the abundance/production rate of sulphur bearing parent molecules and of ethane on the date of S_2 observations, (ii) the precise knowledge of the

deviation, if any, of the number densities of OH and C_2H_4 obtained from Haser's formula from the actual values and (iii) reaction rate coefficients.

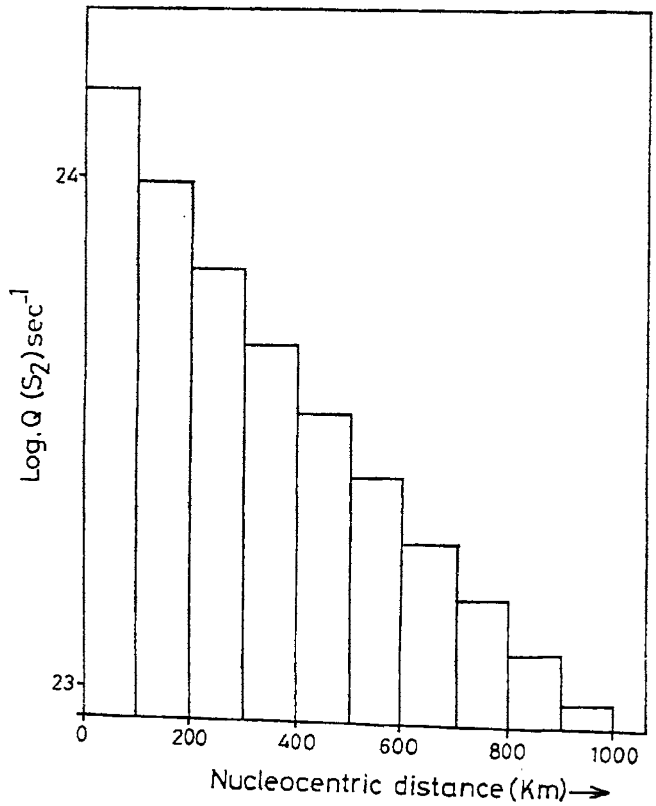

Figure 3. Contribution of the various nucleocentric annular shells towards the total production rate of S_2 molecules in Comet C/1996 B2 (Hyakutake).

8. Conclusions

1. The computed production rate of S_2 molecules in Comet C/1996 B2 (Hyakutake) has been found to be 4.9×10^{24} s^{-1} at 1.06 au. heliocentric distance and agrees well with the observed production rate (6.5 or 10) $\times 10^{24} s^{-1}$ (Laffont *et al.*, 1998) at 0.99 au heliocentric distance, thus putting more confidence in the chemical nature of cometary S_2 molecules.

2. The location of cometary S_2 molecules in Comet C/1996 B2 very near to the nucleus is consistent with the earlier S_2 observations (A'Hearn *et al.*, 1983). Their location in the collision-dominated innermost coma is also consistent with their chemical nature.

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