NEUTRAL TEMPERATURE OF COMETARY ATMOSPHERES

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The spectral analysis of the coma and type I tails of a comet gives a clue to clarify the composition of the volatiles in its nucleus. The ultraviolet observation of strong H, O, and OH emissions in comets 1969 g and i by OAO II (Code and Savage, 1972) and the recent identification of H_2O^+ in the spectrum of 1973f (Wehinger et al., 1974) have suggested that the main constituent of cometary coma is H_2O. It was also suggested from the computation of the ionization processes (Jackson and Donn, 1968) that CO and N_2 may be the second most abundant gases (some ten% by number) in comets. Other gases detected in the optical (C_2, CN, C_3...), ultraviolet (NH, CN) and radio (CH, CH_3, CN) regions appears to be minor constituents of cometary atmospheres.

Water has so large a dipole moment (~ 1.84 Debye) that it is a good infrared radiator. If this molecule is the main constituent of cometary comas, we may expect that the cometary atmosphere may be extremely cooled. This could be the most important factor to determine the neutral temperature of the cometary gas.

Water can emit infrared radiation through a vibrational transition at 6.3 microns and a rotational one near 50 microns. In the vibrational case, the dependence of the emission rate on temperature will mainly be determined by that of the excitation cross-section from $v = 0$ to $v = 1$ level which obeys SSH theory (Schwartz et al, 1952) since the de-excitation rate by molecular collisions is smaller than that of the spontaneous emission (non LTE condition). This rate can be written

$$R_v = 1.2 \times 10^{-22} \, \text{EXP} \, \left(- \frac{38.3}{T^{1/3}} - \frac{2294}{T} \right) N^2 \qquad (1)$$

where T and N are the temperature and density of the cometary gas, respectively.

In the rotational case, the energy differences between adjacent levels are much smaller than those between vibrational ones and so the energy transfer from translational mode to rotational one is much easier. The molecular distribution is of Boltzmann type (LTE condition) and the total emission rate is obtained by summing each contribution over all rotational states. The rotational emission rate of a linear molecule with a dipole moment μ and a rotational constant $\overline{B}$ has been computed by Bates (1951) as

$$R_d = \frac{2^{10} \pi^4}{3} \, c \, \mu^2 \, \overline{B}^4 \left(\frac{k \, T}{hc \, \overline{B}} \right)^2 N \qquad (2)$$

The rotational constants of water are (in cm^{-1}):

$$A = 27.79, \qquad B = 14.51, \qquad C = 9.29.$$

Consequently, by taking $A = \infty$, and $\overline{B} = \sqrt{B\,C}$, an approximate form of emission rate is obtained

$$R_d = 5.5 \times 10^{-19}\ T^2\ N \qquad (3)$$

A better expression for the emission rate of water may be obtained by approximating H_2O as a rigid symmetric rotor ($B = C = \overline{B}$ and $\overline{A} = A$). After some manipulation, the emission rate in this approximation R_r can be written in the form

$$R_r = (1 + \frac{9}{8}\frac{\overline{B}}{\overline{A}} + \frac{3}{8}\frac{\overline{B}}{\overline{A}})\ R_d = 1.54\ R_d \qquad (4)$$

Since the correction factor to the linear dipole approximation is only 50%, the improvement by using a (classical) asymmetric rotor approximation (B≠C) is not very important.

It is noteworthy that the OH radical formed by the dissociation of H_2O has also a large dipole moment and that it may also contribute greatly to the cooling of cometary coma in nearly the same rate as H_2O does, particularly in its outer part. Weaker but still serious contribution may be expected for other radicals such as CN, NH, etc., too.

It may be instructive to compare the planetary upper atmospheres with cometary atmospheres here, since the gas density in the neighborhood of cometary nucleus is around 10^{12} cc, a density similar to those

at the bases of planetary upper atmospheres (although there is a

difference between them in that atmospheric densities of planets

decrease exponentially outwards, while those of comets vary approxi-

mately as the inverse square of the distance). For instance, the cooling

in the Venus and Martian upper atmospheres is due to CO_2 15 micron

band. The heating at the top of these atmospheres by the absorption

of the solar ultraviolet radiation is approximately in balance with the

(vibrational) cooling and their exospheric temperatures become of the

order of some hundreds degrees. For much detailed discussions, some

effects of dynamics (eddy diffusion on the composition of the upper

atmospheres, thermal conduction from heating level to cooling one etc.)

should be taken into account and the inclusion of such effects explained

observed properties of planetary upper atmospheres by space probes

well (Shimizu, 1973a, 1974). Consequently, if the vibrational cooling

due to H_2O 6.3 micron band is the dominant cooling process in the

cometary atmosphere, its neutral gas temperature at 1 AU may also be

around 300 ^{O}K. However, as the formulae (1), (3), and (4) show, the

rotational cooling is much stronger for H_2O. If the heating by the

solar ultraviolet radiation is equated to this, the equilibrium temperature

at 1 AU can be of the order of only 10 ^{O}K. The transport of heat by

expansion of cometary atmosphere can easily be shown to be of the order

of the vibrational cooling and to have a negligible effect as compared

with the rotational one. If the cometary coma has a 300 ^{O}K temperature

it is clear that some other much stronger heating source is necessary

unless H_2O is a minor constituent ($\sim$0.1%) of cometary atmospheres,

which is unlikely from the recent observations. Electron impact may

not be an important source, since a bow shock and other hydromagnetic

structure around a comet may prevent the inflow of such a large electron

energy flux as 10^3 times the ultraviolet radiation into the coma. Consequently,

a possible mechanism may be a strong infrared coupling between H_2O

and dust grain in the coma. It is known that the icy halo model

(Delsemme and Miller, 1971) on the basis of the composition of hydrate

clathrate well explains many observational features including the photo-

dissociation paradox (Wurm, 1963). Recent infrared observations of

comets suggest that the mean radius of cometary dust grain is around

1 micron and that its number density is about 10^7/cc, at least for the

non-volatile part. Even so, the collision time between gas and dust

is much longer than the typical expansion time, $\sim$1 day (although the

collisional times among gases are of the order of 10^{-1} sec, short

enough to be in equilibrium). Consequently about 10^{-2} of the solar

visible radiation, whose energy flux is 10^5 times larger than that in

the ultraviolet region, once absorbed by the dust grain or at the surface

of nucleus should be transferred to H_2O molecules in the form of

infrared radiation. Such a strong infrared coupling could naturally be expected by taking into account that the main part of the dust grain may be H_2O ice, although it is necessary to carry out a tedious radiation transfer problem to obtain the temperature of H_2O gas explicitly.

One of the advantages if this model is that it can explain the dependence of the atmospheric temperature on the distance of comet from the sun, r. Wurm (1963) suggested a relation of $T \propto 1/r$. The heating rate is proportional to N/r^2 and so, if we equate this to (3), T should be inversely proportional to r.

The most important conclusion from the above discussion is that the atmospheric temperature of comets cannot be so high as 1500 ^oK. This is also suspected from the analysis of high resolution CN spectrum (Malaise, 1970). It is concluded from thermochemical calculation (Delsemme, 1966) that the conversion of CH_4 and NH_3 to CO and N_2 occurs at the dissociation level whose temperature is assumed to be extremely high by the absorption of the solar ultraviolet radiation. The expansion of cometary atmosphere is attributed to this heating (Shul'man, 1972) and a detailed hydrodynamic calculation has been carried out on this assumption to support the above quasi-thermochemical equilibrium model (Wallis, 1974). However, all these discussions have

neglected the strong cooling effect of H_2O and should be reconsidered. It is now evident that CO and N_2 may be abundant in the cometary nucleus (Jackson and Donn, 1968), possibly in the form of clathrate. Our proposal in the IAU Symposium No. 52 (Shimizu, 1973b) that the cometary nuclei are composed of the dirty ice of second kind (mainly H_2O and some ten % of CO and N_2) appears to be confirmed. The similarity of cometary molecules to the interstellar molecules should more seriously be taken into account in the theory of cometary formation. Proposals for the origin of comets in interstellar space by Whipple and Lecar and by Donn at this colloquium give a physical meaning to the similarity.

It is to be noted that the ejection of various molecules from stars, both of oxygen rich type (NML Cygnus) and of carbon rich type (IRC + 10216), has been found during these years. Furthermore, CO molecules have been detected in the envelopes of T Tauri stars. This evidence might be correlated with our suggestion for the interchange of cometary substances among stars and clouds, although it is far from conclusive. A large number of interstellar comets trapping the heavy elements appears to be consistent with interstellar deficiences of these elements (Greenberg, 1974).

Addendum: Recent finding of carbon atom emission in the atmosphere

of Comet 1973f (Feldman et al., Science, <u>185</u>, 705, 1974)

endorses the discussion in this paper and this may be a

conclusive evidence for the dirty ice of second kind in

the nuclei of comets.

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DISCUSSION

W. Jackson: If the comets are composed of mostly H_2O, CO and N_2, what is the order of magnitude ratio of $(CO)/(H_2O)$ and $(N_2)/(H_2O)$?

These ratios have to be low if the rate of water evaporation is to control the gas production rate of comets.

M. Shimizu: The composition of volatiles depends on the accretion process and thermal history of comets. I am not discussing them. I tentatively favor clathrate theory, but the real values should be determined by observation.

M. K. Wallis: It is not clear to me that at the relevant cometary densities $(10^6 - 10^8/cm^3)$ and energies, the approach to equilibrium would be rapid enough. Taking H-atoms resulting from photo-dissociation of H_2O with 1-2 eV energy, cooling via rotational excitation with cross-section $10^{-15} cm^2$ and 0.01 eV loss would not dominate elastic collisional transfer of energy from the H-atom to the H_2O. So some energy seems available for increasing the thermal and outflow energies of the H_2O gas. Clearly one has to be careful about drawing definite conclusions one way or the other.

M. Shimizu: The time constant of the excitation is

$$T = \frac{1}{N \; \sigma \; v} = \frac{1}{10^8 \; 10^{-15} \; 10^5} = 10^2 \; sec,$$

much shorter than the expansion time 10^5 sec. So the kinetic energy of hydrogen will be transferred to water, the main constituent, and radiated in the infrared. That leads to the low atmospheric temperature.
(The detailed analysis by taking into account non LTE process and various dynamical effects will be submitted to Astrophysics and Space Science later.)

B. Donn: To try to interpret the radio observations of water in Comet Bradfield, we have worked with Dr. Krauss of the National Bureau of Standards. In a preliminary analysis he obtained a kinetic temperature of 10K in the coma in a similar process to that of Shimizu using cooling by rotational excitation of water. This is clearly an important process to take into account and a detailed analysis is necessary to determine coma temperatures and rotational excitation of molecules.