Distribution of Molecular Hydrogen in the Atmosphere of Titan

J. L. Bertaux

Service d'Aéronomie du Centre National de la Recherche Scientifique

G. Kockarts

Institut d'Aéronomie Spatiale de Belgique

The diffusion problem of light gases in the atmosphere of Titan is reassessed after Voyager encounter. The pre-Voyager theoretical work of Hunten (1973a) is completed by the use of parameters derived from Voyager encounter: the radial distances of turbopause level (3500 km) and critical level (4100 km), the exospheric temperature (186 K) and the volume mixing ratio of 2×10^{-3} for H_2. An analytical expression of the solution of the diffusion equation is given for a spherical geometry and an isothermal atmosphere. It is used to predict an altitude profile of H_2 in the upper atmosphere of Titan. The modification of this profile by a possible return flow of H_2 from a torus to the atmosphere of Titan is addressed, and is found negligible since there is observational evidence from Voyager that the H_2 density is less than 100 cm^{-3} in the torus, at large distance from Titan. The H_2 concentration at the exobase level is 3.1×10^5 cm^{-3}, and the thermal escape of H_2 is nearly equal to the diffusion limiting flux of 3.4×10^9 molecules cm^{-2} s^{-1} at the turbopause level. Photodissociation of CH_4 has to provide for an equal constant supply of H_2.

1. Introduction

Methane was the first gas identified by *Kuiper* [1944] as a component of Titan's atmosphere. *Trafton* [1972] discovered an absorption feature in the near infrared around 815 nm and he tentatively attributed it to the 3-0 S(1) quadrupole line of molecular hydrogen with an abundance of the order of 5 km-atm corresponding to a H_2 total content of 1.4×10^{25} cm^{-2}. Although this interpretation has been seriously questioned [see *Owen*, 1982], it stimulated an important study of the diffusion and escape of H_2 by *Hunten* [1973a], who showed that a pure atmosphere of 5 km-atm of H_2 would last only for a few hours. An additional heavier gas was necessary to retain such a large amount of H_2, and *Hunten* [1973a] suggested N_2 and CH_4 as possible candidates. This brilliant prediction was later confirmed by VOYAGER 1 [*Hanel et al.*, 1981]. Besides the major constituents N_2 and CH_4, many hydrogen compounds have been detected in the infrared as trace species [*Hanel et al.*, 1981] and H_2 has been identified in the lower atmosphere with a volume mixing ratio of 0.002 ± 0.001 [*Samuelson et al.*, 1981] equivalent to 0.2 km-atm, i.e. a value far less than the estimation of *Trafton* [1972]. Furthermore, an atomic hydrogen torus surrounding Saturn near the orbit of Titan has been discovered by *Broadfoot et al.* [1981] and it is assumed to be fed by escape from the upper atmosphere of Titan.

Using the atmospheric model of *Smith et al.* [1982], we deduce in the present paper a vertical distribution of H_2 throughout Titan's atmosphere. The general atmospheric background, including possible exospheric distributions, is presented in section 2. The diffusion equation is solved analytically in section 3 for a spherical geometry taking into account the variation of gravity with altitude. The H_2 distribution is presented in section 4 and it is discussed in relation with the possible existence of a molecular hydrogen torus.

2. Atmospheric Composition and Structure

·Our knowledge of Titan's atmosphere results essentially from three experiments on board VOYAGER 1: the infrared interferometer (IRIS), the ultraviolet spectrometer (UVS), and the radio science occultation measurements. The major component is N_2 with a volume mixing ratio of 0.87 ± 0.07 and the total ground level pressure is 1.6 bar with a temperature of 95 ± 2 K [*Hanel et al.*, 1981; *Tyler et al.*, 1981; *Samuelson et al.*, 1981; *Owen*, 1982]. Furthermore, the N_2 abundance is measured with the UVS by solar occultation in the upper atmosphere between 3700 − 4100 km radial distance, and the temperature is estimated to be 186 ± 20 K [*Smith et al.*, 1982]. This value is 21 K higher than the temperature deduced from IRIS around 2750 km radial distance [*Hanel et al.*, 1981].

The molecular nitrogen concentration $n(r)$ at radial distance r is given by an isothermal hydrostatic distribution such as

$$n(r) = n(r_0)e^{-E(1-y)} \qquad (1)$$

where $y = r_0/r$ and $E = r_0/H_0$ with H_0 being the partial pressure scale height of N_2 at the reference level r_0. The N_2 model used in the present paper is identical to the engineering model developed by *Smith et al.* [1982]. We have, therefore, considered two isothermal zones in which (1) is applied with the following conditions:

1. Between 2750 and 3840 km, $T = 165$ K and at 2750 km, $n(N_2) = 4.4 \times 10^{16}$ cm^{-3}, $H_0 = 41.27$ km, and $E = 66.63$

2. Above 3840 km, $T = 186$ K and at 3840 km, $n(N_2) = 2.7 \times 10^8$ cm^{-3}, $H_0 = 90.72$ km, and $E = 42.33$.

The increase in the scale height H between 2750 km and 3840 km radial distance essentially results from the decrease in the acceleration of gravity.

From the hydrocarbon density distribution, analyzed with a simple photochemical model, *Smith et al.* [1982] deduced a turbopause level at 3500 ± 70 km radial distance. With a value of 2575 ± 2 km for Titan's radius [*Lindal et al.*, 1981] the turbopause is at 925 ± 70 km altitude. We will, however,
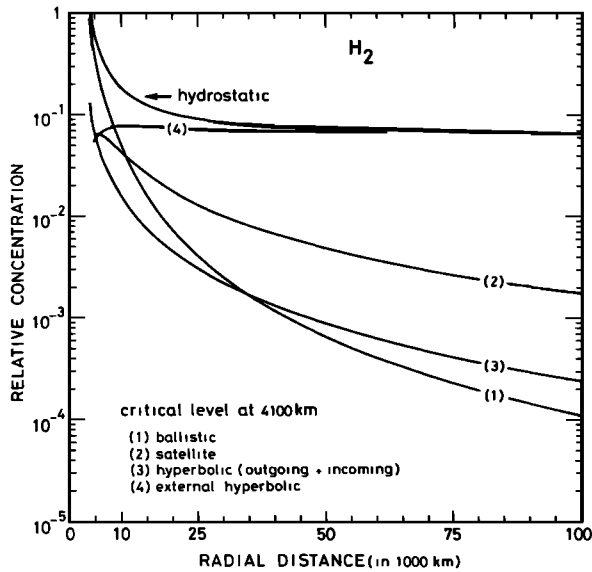
Fig. 1. Molecular hydrogen relative distribution as a function of radial distance. Temperature at the critical level is 186 K. When all particles labelled (1), (2), (3), and (4) are present, their sum leads to a hydrostatic distribution in Titan's exosphere.

explore a slightly larger range of the turbopause level in order to examine its influence on the H_2 distribution.

A complete description of an upper atmosphere requires also a knowledge of the radial distance r_c of the exobase or critical level. It has been shown by *Banks and Kockarts* [1973] that the critical level is not a sharp transition between the heterosphere and the exosphere, but merely is the level where the probability for a particle with velocity greater than the escape velocity has a certain value. According to equation (16.61) of *Banks and Kockarts* [1973] a critical level for a constituent 1 defined bv

$$\sum_i n_i H_i Q_{1i} = 1 \tag{2}$$

corresponds to a probability e^{-1} for an infinite free path. In equation (2) the summation extends over all constituents i with concentrations n_i, partial pressure scale heights H_i and collision cross sections Q_{1i}. When equation (2) is applied to H_2 molecules colliding with N_2 and CH_4 in Titan's atmosphere, one obtains a critical level around 4100 km radial distance for a temperature of 186 K and with the collision cross sections used by *Hunten* [1973a].

The effusion velocity w_c used in the computation of Jeans' thermal escape can be written

$$w_c = (kT/2\pi m)^{1/2}(1 + E_c)e^{-E_c} \tag{3}$$

where k is Boltzmann's constant, T is the temperature at the critical level, m is the molecular mass of the escaping constituent, and $E_c = r_c/H_c$ at the critical level. It is interesting to note that with equation (3) and with a hydrostatic distribution of the escaping particles, the value of the escape flux does not strongly depend on the altitude of the critical level. From expression (16.65) of *Banks and Kockarts* [1973], it appears that an exobase at (4100 ± 100) km radial distance leads to a Jeans' escape flux $F_c = F_{4100} \times (1 \pm 0.02)$ for H_2.

Since the effusion velocity given by equation (3) is 7.9 × 10^3 cm s^{-1} at 4100 km for $T = 186$ K, a relatively large escape flux is expected for H_2. A Saturnian torus of atomic hydro-

gen, centered on the orbit of Titan was actually discovered by *Broadfoot et al.* [1981] with a concentration of the order of 20 atoms cm^{-3}. A torus of molecular hydrogen could also exist with a much higher concentration, since H_2 is notoriously more difficult to detect than the Lyman-α emission of atomic hydrogen. It is even possible that a return flow of H_2 from the torus enters in the upper atmosphere of Titan. The extreme situation would be characterized by a return flux equal to Jeans' thermal escape at the critical level, leading to a net flux equal to zero at all levels. This would be a hydrostatic exosphere in which the outgoing flux is exactly compensated by the incoming flux of hyperbolic particles.

In a classical exosphere [*Chamberlain*, 1963], composed of ballistic particles, which return to the critical level, and hyperbolic particles, which escape, the velocity distribution function at any given point in the exosphere is an incomplete Maxwellian distribution. It is, however, possible to add the necessary particles to obtain a complete Maxwellian distribution. This implies the existence of satellite particles, hyperbolic particles crossing the critical but coming from interplanetary space and external hyperbolic particles that never cross the exobase. *Banks and Kockarts* [1973] have given simple analytical expressions in their equations (16.49) to (16.52) for the computation of the vertical distribution of each type of particles. Figure 1 gives these distributions for H_2. The concentrations are normalized to unity at the critical level where the temperature is 186 K. At large distance the hydrostatic distribution essentially results from the external hyperbolic particles. The outgoing and incoming hyperbolic particles are present in equal amount, so that the escape flux is exactly balanced by a return flux. If such a situation exists, the relative contribution of the return flux to the concentration at the critical level is 6.4% for H_2. An absolute estimate would require a measurement of the hyperbolic incoming particles at large distance of Titan. Another simpler estimate is, however, possible in the case of a hydrostatic exosphere in which the H_2 concentration would be given by (1), with $E = E_c = 2.84$. In such an extreme situation, a knowledge of the H_2 concentration in the torus very far from Titan allows a direct computation of the contribution to the critical level concentration by use of a hydrostatic distribution. The equality between outgoing and incoming fluxes allows then to make use of the effusion velocity (3) to compute the return flow. Such a procedure leads to an upper limit that is evaluated in section 4 after the presentation of the analytical solution for the diffusion equation in the next section.

3. DIFFUSION EQUATION

When a light gas with concentration n_1 diffuses through an isothermal background atmosphere with no vertical wind, the diffusion velocity $w_1(r)$ can be written [*Banks and Kockarts*, 1973] as

$$w_1(r) = -D\left(\frac{1}{n_1}\frac{dn_1}{dr} + \frac{1}{H_1}\right) - K\left(\frac{1}{n_1}\frac{dn_1}{dr} + \frac{1}{H}\right) \tag{4}$$

where D and K are the molecular diffusion coefficient and the eddy diffusion coefficient, respectively, $H_1 = kT/m_1 g$ is the partial pressure scale height of the light gas, and H is the pressure scale height for the background gas. Above the turbopause level K can be considered as negligible so that (4) becomes

$$w_1(r) = -D\left(\frac{1}{n_1}\frac{dn_1}{dr} + \frac{1}{H_1}\right) \qquad (5)$$

which is equivalent to equation (A9) of *Hunten* [1973b]. When chemical production and loss terms are ignored or compensate each other, the continuity equation in spherical coordinates leads to

$$r^2 n_1 w_1 = r_0^2 \phi_0 \qquad (6)$$

where ϕ_0 is the flux at a reference level r_0. This implies that the surface integrated flux $4\pi r^2 \phi(r)$ is constant throughout the atmosphere, but not the local flux $\phi(r)$. The diffusion equation (5) can now be written as

$$D\left(\frac{dn_1}{dr} + \frac{n_1}{H}\right) = -(r_0/r)^2 \phi_0 \qquad (7)$$

where the molecular diffusion coefficient of a minor constituent diffusing through N_2 is given by

$$D = D_0 n_0(N_2)/n(N_2) \qquad (8)$$

D_0 being its value at the reference level r_0. Making a change of variable $y = r_0/r$, it is easily seen that

$$1/H_1 = E_1(r_0/r^2) \qquad (9)$$

with $E_1 = r_0/H_{10}$. The parameter E_1 for the minor constituent with mass m_1 is related to the parameter E for the background gas with mass m by

$$E = E_1(m/m_1) \qquad (10)$$

Using for N_2 the hydrostatic expression (1), the diffusion equation (7) is transformed into

$$\frac{dn_1}{dy} - n_1 E_1 = (r_0 \phi_0/D_0)e^{-E(1-y)} \qquad (11)$$

This first order differential equation can be integrated analytically and its solution is

$$n_1 = \frac{r_0 \phi_0}{D_0(E - E_1)} e^{-E(1-y)} + n_{10}$$

$$\cdot \left\{1 - \frac{r_0 \phi_0}{D_0(E - E_1)n_{10}}\right\} e^{-E_1(1-y)} \qquad (12)$$

where n_{10} is the concentration at the reference level r_0 where $y = 1$. This is actually the boundary condition and from a mathematical point of view ϕ_0 is a free parameter that will influence the shape of the distribution. The solution (12) can be obtained also from the more general expressions given by *Kockarts* [1973].

For the case of a plane parallel atmosphere with no variation of gravity, *Hunten* [1973a] showed that the diffusion equation has a solution with two components, one with the background scale height and one with the partial pressure scale height of the minor diffusing constituent. Such a situation is also found in (12) valid for spherical geometry and height dependent gravity acceleration. Furthermore, two extreme cases appear in the solution (12). If the flux $\phi_0 = 0$, the solution (12) reduces to a hydrostatic distribution with scale height H_{10} for constituent 1. If, however, ϕ_0 is given exactly by the limiting flow

$$\phi_0 = \frac{D_0}{H}\left(1 - \frac{m_1}{m}\right)n_{10} = D_0\left(\frac{1}{H_0} - \frac{1}{H_{10}}\right)n_{10} \qquad (13)$$

the solution (12) reduces to a perfect mixing distribution $n_1 = n_{10} \exp[-E(1 - y)]$ with scale height H_0, since in that case $r_0 \phi_0/[D_0(E - E_1)] = n_{10}$. This implies that, for any distribution between these two extreme cases, the actual diffusion velocity is always smaller (even very slightly) than the maximum diffusion velocity involved in (13).

4. MOLECULAR HYDROGEN DISTRIBUTION

In the model atmosphere of *Smith et al.* [1982], the temperature is 165 K between the turbopause level r_t and a level r_a at 3840 km radial distance and it abruptly changes to 186 K between r_a and the critical level r_c. Equation (12) must, therefore, be applied with some caution. When the critical level is taken as the reference level, (12) completely determines the shape of the profile $n_1(r)/n_{1c}$ and the ratio $n_1(r_a)/n_{1c}$ at 3840 km radial distance. Since the effusion velocity is given by (3), the conservation of the surface integrated flux, leads to a determination of the diffusion velocity $w(r_a)$ from $r_a^2 n_1(r_a)w(r_a) = r_c^2 n_{1c}w_c$. Equation (12) can then be applied a second time with $r_a = 3840$ km between r_a and the turbopause level. The shape of the H_2 profile is thus obtained between r_t and r_a. For H_2 the binary diffusion coefficient D_0 has been taken from *Hunten* [1973a] as $n_0(N_2)D_0 = 1.88 \times 10^{17} T^{0.82}$ (cm^{-1} s^{-1}). With a molecular nitrogen concentration of 2.77×10^{10} cm^{-3} at 3500 km radial distance and a measured volume mixing ratio [*Samuelson et al.*, 1981] of 2×10^{-3} for H_2, we obtain the molecular hydrogen distribution shown in Figure 2. The N_2 distribution
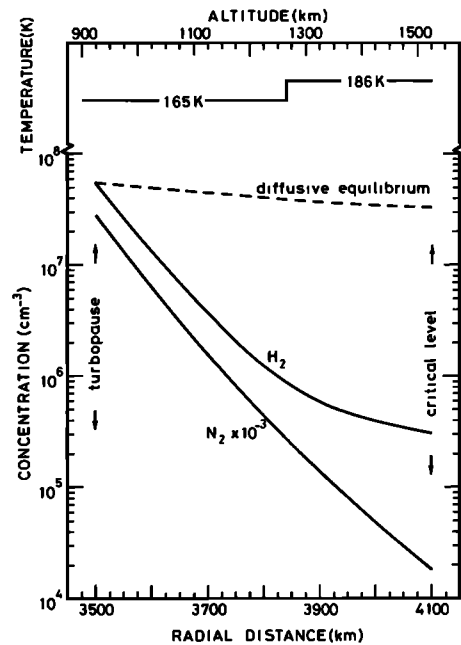

Fig. 2. Vertical distribution of N_2 and H_2 as a function of radial distance (lower scale) and altitude (upper scale) when Titan's radius is 2575 km. The turbopause and the exobase (or critical level) are indicated by vertical arrows. H_2 volume mixing ratio at the turbopause is 2×10^{-3}. The dashed curve corresponds to diffusive equilibrium distribution for which the net transport flux is zero. This situation can occur when the exospheric incoming flux or return flux is equal to Jeans' thermal escape. The temperature distribution is shown in the upper part of this figure.

is also indicated and the dashed curve corresponds to a H$_2$ distribution in diffusive equilibrium with $\phi_0 = 0$ in equation (12). The Jeans' escape flux for H$_2$ is $\phi_c = 2.47 \times 10^9$ cm^{-2} s^{-1} and the surface integrated flux at 4100 km radial distance is $F_c = 4\pi r_c^2 \phi_c = 5.22 \times 10^{27}$ molecules per second, i.e., a value comparable to the production rate of a modest comet at 1 AU. The corresponding local flux at the turbopause is $\phi_t = \phi_c (r_c/r_t)^2 = 1.372 \phi_c = 3.39 \times 10^9$ cm^{-2} s^{-1}. The maximum diffusive flux or limiting flux given by (13) is 3.44 $\times 10^9$ cm^{-2} s^{-1}, i.e., a value only 1.5% larger than the escape flux referred to the turbopause level. This explains why the slope of the H$_2$ profile is almost identical to the slope of the background gas N$_2$ as can be seen in Figure 2 around the turbopause. The effect of an arbitrary variation of the turbopause level from 3300 km to 3700 km radial distance indicates that a shift of ±200 km around the radial distance of 3500 km does not produce a variation larger than 10% in the H$_2$ concentration at the critical level. In our computation we have neglected the photochemistry recently reviewed by Strobel [1982] since the solar radiation which photodissociates CH$_4$ is mainly absorbed below the turbopause level where we have adopted the measured volume mixing ratio of 2 $\times 10^{-3}$ for H$_2$.

The escape flux of 2.47 $\times 10^9$ cm^{-2} s^{-1} corresponds to a surface level flux of 6.26 $\times 10^9$ cm^{-2} s^{-1}. A H$_2$ mixing ratio of 2 $\times 10^{-3}$ corresponds to a column content of 5.13 $\times 10^{23}$ cm^{-2} at the surface of Titan where the atmospheric scale height is 20.4 km. The time constant for evacuating the whole H$_2$ content of Titan's atmosphere is, therefore, 8.2 $\times 10^{13}$ s. Without a continuous supply, the H$_2$ content would be eliminated in 2.6 million years. However, Strobel [1982] has shown that the rate of hydrogen production in all forms leads to a flux of the order of 1.4 $\times 10^{10}$ cm^{-2} s^{-1} at the turbopause. This value is sufficient to compensate the molecular hydrogen upward flux of 3.39 $\times 10^9$ cm^{-2} s^{-1} at 3500 km radial distance.

The question of a possible effect of a return flow was addressed by Hunten [1977] during the pre-Voyager period. In order to examine the possible contribution from a molecular hydrogen torus to the concentration of H$_2$ below the critical level, we need an estimate of H$_2$ in the torus. W.-H. Ip (unpublished manuscript, 1982) indirectly derived an upper limit from the low energy charged particles (LECP) instrument, which detected a flow of 4.3 cm^{-2} s^{-1} energetic neutral particles at an upstream distance of 45 Saturnian radii [Kirsch et al., 1981]. The most likely source of these neutrals is charge exchange of magnetospheric protons with H atoms or H$_2$ molecules. An upper limit of 1.6 $\times 10^2$ cm^{-3} was deduced by W.-H. Ip (unpublished manuscript, 1982) and we will retain a molecular hydrogen concentration of 10^2 as a reasonable value in the torus.

We have shown in section 2 that a hydrostatic exosphere implies an exact balance between outgoing and incoming fluxes. Since the concentration distribution is then given by equation (1) with $E = E_c = 2.84$ for H$_2$, a value of 10^2 cm^{-3} H$_2$ molecules at sufficiently large distance where $y = r_0/r \cong 0$ leads to a concentration of 1.7 $\times 10^3$ cm^{-3} at the critical level, i.e. only 0.5% of the H$_2$ population shown at 4100 km radial distance in Figure 2. The return flow is then given by the classical Jean's expression $F_c = 4\pi r_c^2 w_c \times 1.7 \times 10^3 = 2.8 \times 10^{25}$ molecules per second. This value is negligible compared to the thermal escape of 5.22 $\times 10^{27}$ molecules per second. As a consequence, the H$_2$ component corresponding

to a torus population of 100 cm^{-3} can be ignored in the atmosphere of Titan below the critical level.

5. CONCLUSION

An analytical solution of the diffusion equation for a spherical geometry and an isothermal atmosphere provides a vertical profile of molecular hydrogen when physical parameters measured during Voyager encounter with Titan's atmosphere are used. The H$_2$ concentration varies from 5.5 $\times 10^7$ cm^{-3} at a turbopause radial distance of 3500 km to 3.1 $\times 10^5$ cm^{-3} at a critical level of 4100 km radial distance where the escape flux is 2.5 $\times 10^9$ cm^{-2} s^{-1}. The importance of the escape flux is such that a variation of ±200 km of the turbopause level does not change the concentration at the critical level by more than 10%. The observed existence of an atomic hydrogen torus leads to an estimation of the concentration of a molecular hydrogen torus that has not yet been detected. The estimated concentration of H$_2$ in the torus is 100 cm^{-3}. When the effect of a return flow from the torus toward Titan's atmosphere is evaluated in a hydrostatic exosphere, it appears that the contribution of the torus to the H$_2$ concentration below the critical level is negligible.

REFERENCES

Banks, P. M. and G. Kockarts, Aeronomy, Part A and Part B, Academic Press, New York, 1973.

Broadfoot, A. L., B. R. Sandel, D. E. Shemansky, J. B. Holberg, G. R. Smith, D. F. Strobel, J. C. McConnell, S. Kumar, D. M. Hunten, S. K. Atreya, T. M. Donahue, H. W. Moos, J. L. Bertaux, J. E. Blamont, R. B. Pomphrey and S. Linick, Extreme ultraviolet observations from Voyager 1 encounter with Saturn, Science, 212, 206–211, 1981.

Chamberlain, J. W., Planetary coronae and atmospheric evaporation, Planet. Space Sci., 11, 901–960, 1963.

Hanel, R., B. Conrath, F. M. Flasar, V. Kunde, W. Maguire, J. Pearl, J. Pirraglia, R. Samuelson, L. Herath, M. Allison, D. Cruikshank, D. Gautier, P. Gierasch, L. Horn, R. Koppany and C. Ponnamperuma, Infrared observations of the Saturnian system from Voyager 1, Science, 212, 192–200, 1981.

Hunten, D. M., The escape of H$_2$ from Titan, J. Atmos. Sci., 30, 726–732, 1973a.

Hunten, D. M., The escape of light gases from planetary atmospheres, J. Atmos. Sci., 30, 1481–1494, 1973b.

Hunten, D. M., Titan's atmosphere and surface, in Planetary Satellites, edited by J. A. Burns, pp. 420–437, University of Arizona Press, Tucson, 1977.

Kirsch, E., S. M. Krimigis, W. H. Ip, and G. Gloeckler, X ray and energetic neutral particle emission from Saturn's magnetosphere, Nature, 292, 718–721, 1981.

Kockarts, G., Helium in the terrestrial atmosphere, Space Sci. Rev., 14, 723–757, 1973.

Kuiper, G. P., Titan: A satellite with an atmosphere, Astrophys. J., 100, 378–383, 1944.

Lindal, G. F., H. B. Hotz, D. N. Sweetnam, V. R. Eshleman, and G. L. Tyler, The atmosphere of Titan: An analysis of the Voyager 1 radio occultation measurements, Bull. Am. Astron. Soc., 13, 700–701, 1981.

Owen, T., The composition and origin of Titan's atmosphere, Planet. Space Sci., 30, 833–838, 1982.

Samuelson, R. E., R. A. Hanel, V. G. Kunde, and W. C. Maguire, Mean molecular weight and hydrogen abundance of Titan's atmosphere, Nature, 292, 688–693, 1981.

Smith, G. R., D. F. Strobel, A. L. Broadfoot, B. R. Sandel, D. E. Shemansky, and J. B. Holberg, Titan's upper atmosphere: Composition and temperature from the EUV solar occultation results, J. Geophys. Res., 87, 1351–1357, 1982.

Strobel, D. F., Chemistry and evolution of Titan's atmosphere, *Planet. Space Sci., 30,* 839–848, 1982.

Trafton, L., On the possible detection of H_2 in Titan's atmosphere, *Astrophys. J., 175,* 285–293, 1972.

Tyler, G. L., V. R. Eshleman, J. D. Anderson, G. S. Levy, G. F. Lindal, G. E. Wood, and T. A. Croft, Radio science investigations of the Saturn system with Voyager 1: Preliminary results, *Science, 212,* 201–206, 1981.

J. L. Bertaux, Service d'Aéronomie du Centre National de la Recherche Scientifique, F-91370 Verrières-le-Buisson, France.

G. Kockarts, Institut d'Aéronomie Spatiale de Belgique, 3 avenue Circulaire, B-1180, Brussels, Belgium.