

## PHOTOIONIZATION AND PHOTODISSOCIATION IN DIFFUSE INTERSTELLAR CLOUDS

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### ABSTRACT

An accurate treatment of radiative transfer is used to explore the effects of grain scattering properties on the photoionization and photodissociation efficiencies of atomic and molecular constituents in diffuse clouds and to calculate the rates of heat deposition by photoelectric emission from grains. The observational data on ionization and dissociation are consistent with, but do not establish, a grain scattering model which is highly anisotropic at short wavelengths.

*Subject headings:* atomic processes — interstellar: matter — molecular processes — radiative transfer

### I. INTRODUCTION

The ultraviolet radiation field is a critical parameter in the determination of the thermal and ionization balance, the chemistry, the stability, and the evolution of diffuse interstellar clouds. It determines in particular the heating by photoelectric emission from the dust grains and the efficiencies of photodestruction of the atomic and molecular constituents of the clouds. The radiation field in the clouds is modified by scattering and absorption due to dust grains which provide the major source of continuum opacity.

The influence of the scattering properties of the grains on molecular lifetimes in dense clouds has been explored by Sandell and Mattila (1975); Whitworth (1975); Bernes and Sandqvist (1977); and Sandell (1978) who showed that the lifetimes are sensitive to the anisotropy of the scattering phase function and to the albedo. At ultraviolet wavelengths, both the scattering phase function and the albedo are highly uncertain (cf. Jura 1979).

In this paper we employ an accurate treatment of radiative transfer (Flannery, Roberge, and Rybicki 1980) to examine the physical consequences of anisotropic, coherent, nonconservative grain scattering in diffuse interstellar clouds with visual extinctions  $A_v$  less than unity. We calculate the rates of photoionization of the atomic constituents as a function of optical depth. From a comparison of the results of different models, we conclude that the observations are consistent with grains whose extinction at wavelengths  $\lambda < 2000 \text{ \AA}$  is dominated by forward scattering but do not exclude scattering with little anisotropy.

We carry out a similar analysis of the photodissociation rates of interstellar molecules for diffuse clouds. In agreement with earlier studies (Sandell and Mattila 1975; Sandell 1978), we find that with increasing optical depth the molecular lifetimes become very sensitive to the degree of anisotropy. For forward scattering, photodissociation is a significant destruction mechanism deep into molecular clouds.

The scattering properties also exert an important influence on the heat deposition in clouds arising from the photoelectric effect on grains.

### II. THE ULTRAVIOLET RADIATION FIELD AND GRAIN PROPERTIES

We consider semi-infinite plane parallel clouds with visual extinctions less than unity. Stars and other localized sources of ionizing radiation are assumed to be sufficiently distant that their influence is negligible. The radiation inside our model clouds originates at both surfaces, which are illuminated isotropically with intensity  $I_\lambda^0$  at wavelength  $\lambda$  by the average interstellar radiation field. Then the specific intensity  $I_\lambda(\tau_\lambda, \mu)$  at optical depth  $\tau_\lambda$  and at an angle  $\cos^{-1} \mu$  with respect to the "upward" normal is the solution to the usual equation of radiative transfer

$$\mu \frac{\partial I_\lambda}{\partial \tau_\lambda} = I_\lambda - S_\lambda \quad (1)$$

and the appropriate boundary conditions are

$$I_\lambda(\tau_\lambda = 0, \mu < 0) = I_\lambda^0, \quad (2a)$$

$$I_\lambda(\tau_\lambda = 2T_\lambda, \mu > 0) = I_\lambda^0, \quad (2b)$$

where  $T_\lambda$  is the optical depth to the center of the cloud.

We assume that radiative transfer occurs solely by coherent, nonconservative, anisotropic scattering by dust grains, and we ignore emission and absorption by the gas. At the low temperatures of interstellar clouds, thermal emission in the ultraviolet is negligible; but in clouds of sufficient density and opacity, continuum absorption by neutral carbon atoms will increase the lifetimes of molecules such as  $\text{H}_2\text{CO}$ , OH, and CO (Myers and Ho 1975; Bernes and Sandqvist 1977; Sandell 1978). However, for clouds with  $A_v < 1$ , the column density of neutral carbon is not more than  $4 \times 10^{15} \text{ cm}^{-2}$  (Morton 1975; Snow 1976, 1977). The photoionization cross section of carbon is  $1.7 \times 10^{-17} \text{ cm}^2$  (Taylor and Burke

1976; Hofmann and Trefitz 1980) so that the optical depth is not more than 0.06 and the screening effect is unimportant.

Line absorption by molecular hydrogen is a complicating factor at wavelengths shorter than 1108 Å which particularly affects the photoionization of carbon whose ionization threshold lies at 1101 Å and possibly of chlorine and ionized calcium whose ionization thresholds lie at 956 Å and 1045 Å, respectively. According to Black and Dalgarno (1977), H<sub>2</sub> line absorption reduces the carbon photoionization rates by about 25% in the case of isotropic grain scattering. The effect will be larger for grains which scatter preferentially in the forward direction, and detailed calculations for specific clouds may be necessary. Here we note merely that because of our neglect of H<sub>2</sub> line absorption the calculated photoionization rates of carbon, chlorine, and ionized calcium are too large.

With these simplifications,  $\tau_\lambda$  is simply the optical depth for dust extinction at wavelength  $\lambda$ . The source function  $S_\lambda$  in equation (1) is due to scattering by dust with albedo  $\omega_\lambda$  and phase function  $p_\lambda(\mu', \mu)$ . Thus,

$$S_\lambda = \frac{\omega_\lambda}{2} \int_{-1}^{+1} I_\lambda(\mu') p_\lambda(\mu', \mu) d\mu' \quad (3)$$

where  $\mu'$  and  $\mu$  specify the directions of the incident and scattered photons, respectively. For  $p_\lambda$  we adopt the azimuthally symmetric, one-parameter representation of Henyey and Greenstein (1941),

$$p_\lambda(\mu', \mu) = \sum_{l=0}^{\infty} (2l+1) g_\lambda {}^l P_l(\mu) P_l(\mu'), \quad (4)$$

where  $P_l$  is the Legendre polynomial of order  $l$ . The asymmetry parameter  $g_\lambda$  varies from zero for isotropic scattering to unity for scattering that is completely forward.

We specify  $I_\lambda$  and the rates of all processes as functions of optical depth in the visual band,  $\tau_v$ , measured from the upper surface of the cloud to the center at  $T_v$ . All quantities are therefore completely determined by  $T_v$  and the four functions of wavelength,  $x_\lambda = \tau_\lambda/\tau_v$ ,  $\omega_\lambda$ ,  $g_\lambda$ , and  $I_\lambda^0$ .

The function  $x_\lambda$  can be written in terms of observable quantities as

$$x_\lambda = \frac{1}{R_v} \frac{E(\lambda - V)}{E(B - V)} + 1 \quad (5)$$

Extinction curves have been measured for numerous stars at wavelengths down to  $\lambda = 1000$  Å (Bless and Savage 1972; York *et al.* 1973; Snow 1976). Variations from star to star are large, and we have adopted the averaged values of  $x_\lambda$  shown in Figure 1a which for  $\lambda > 1000$  Å is the average extinction curve of Bless and Savage (1972). The extrapolation to shorter wavelengths is plausible but arbitrary.

The albedo  $\omega_\lambda$  and asymmetry parameter  $g_\lambda$  can be inferred from measurements of the light scattered by dust grains by using radiative transfer models that reproduce

the data. This procedure has been applied to observations of the diffuse galactic light (Lillie and Witt 1976) and to observations of reflection nebulae for  $\lambda \geq 1500$  Å (Andriesse, Piersma, and Witt 1977; Witt 1977) with conflicting results. The diffuse galactic light observations are reproduced by models in which grain scattering is forward peaked in the ultraviolet, but the observations of the reflection nebula 23 Tau are consistent with models in which scattering is isotropic at 1550 Å. Although the case is less clear with regard to  $\omega_\lambda$ , similar problems may exist.

Recent attempts to resolve the discrepancy in the values of  $g_\lambda$  have been unsuccessful. New observations (Morgan, Nandy, and Thompson 1978; Witt and Cottrell 1979) and a reanalysis of the old data (Jura 1979) confirm the conflict. The conflict might be resolved by an appropriate choice of the geometry of dust and stars in reflection nebulae. Radiative transfer models contain four parameters in addition to  $\omega_\lambda$  and  $g_\lambda$  (Andriesse, Piersma, and Witt 1977), and the studies have not exhausted the entire parameter space. Alternatively, more than one kind of grain may occur in the different physical environments.

We present results for three models of  $\omega_\lambda$  (Fig. 1b) and  $g_\lambda$  (Fig. 1c) which span the range of values allowed by observations. For  $\lambda \geq 1550$  Å, models 2 and 3 are identical and are consistent with observations of the diffuse galactic light, whereas model 1 is consistent with observations of reflection nebulae. For  $\lambda < 1550$  Å, we employ different extrapolations for the three cases, which should span the range of possibilities. There is some evidence that models 2 and 3, for which  $\omega_\lambda$  and  $g_\lambda$  are large, are more appropriate (Carruthers and Opal 1977; Henry *et al.* 1978).

The illuminating intensity  $I_\lambda^0$  depends on the height of the cloud above the galactic plane and on its proximity to hot stars (Jura 1974). Our models apply to clouds in the galactic plane far from ionizing sources. Then  $I_\lambda^0 = 0$  for  $\lambda < 912$  Å. At longer wavelengths between 912 Å and 2400 Å, we use

$$I_\lambda^0 = 5.1 \times 10^6 \lambda^{-4} - 8.1 \times 10^9 \lambda^{-5} + 3.2 \times 10^2 \lambda^{-6} \quad (6)$$

measured in units of ergs cm<sup>-2</sup> s<sup>-1</sup> ster<sup>-1</sup> Å<sup>-1</sup> (Draine 1978), which is a fit to theoretical estimates of  $I_\lambda^0$  in spiral arms (Habing 1968; Gondhalekar and Wilson 1975) and the solar neighborhood (Witt and Johnson 1973; Jura 1974), as well as to measurements of its local value (Hayakawa, Yamashita, and Yoshioka 1969; Belyaev *et al.* 1970; Henry *et al.* 1977). For  $\lambda > 2400$  Å, equation (6) was extrapolated to agree with the data of Witt and Johnson (1973). The values of  $I_\lambda^0$  are given in Figure 1d.

Equations (1) through (4) were solved for  $I_\lambda$  by the method of spherical harmonics (Flannery, Roberge, and Rybicki 1980). In the method, the mean intensity

$$J_\lambda(\tau_v) = \int_{-1}^{+1} I(\tau_v, \mu) d\mu \quad (7)$$

is given by

$$J_\lambda(\tau_v) = \sum_{m=1}^M A_m \{ \exp(-k_m \tau_v) + \exp[k_m(\tau_v - 2T_v)] \}, \quad (8)$$

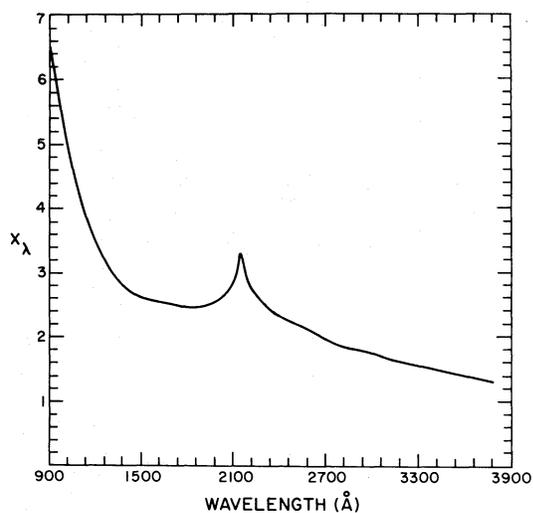


FIG. 1a

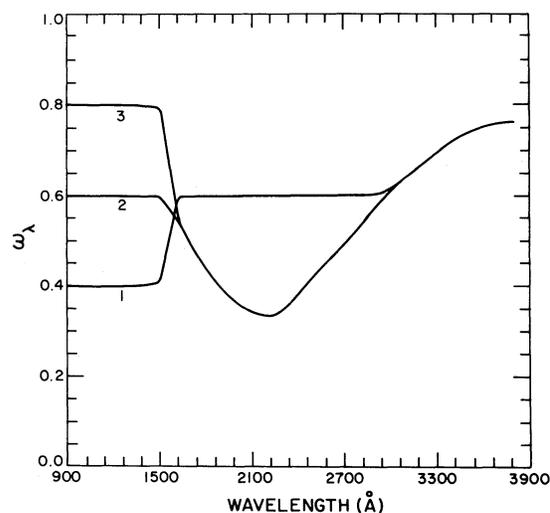


FIG. 1b

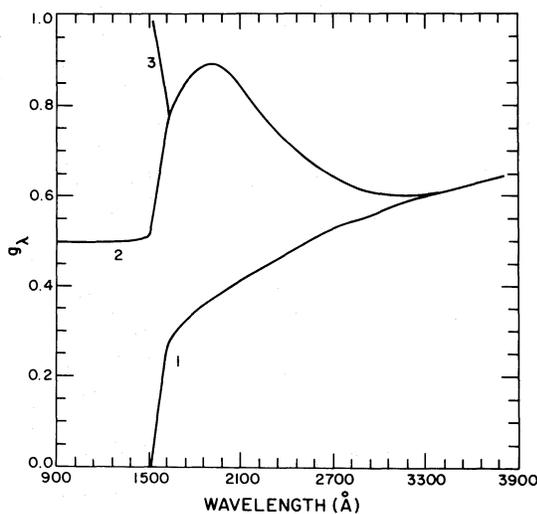


FIG. 1c

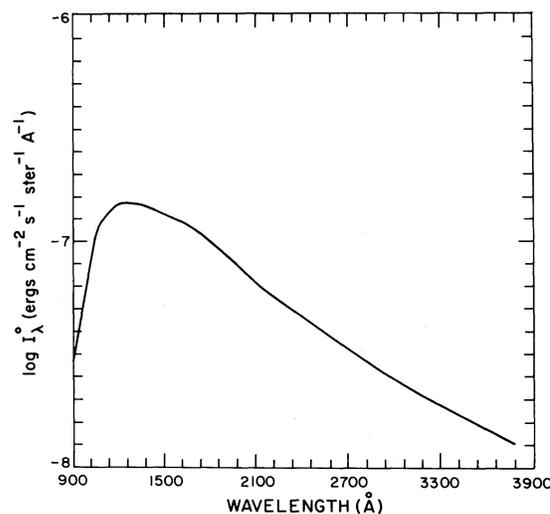


FIG. 1d

FIG. 1.—(a) Values of  $x_\lambda = \tau_\lambda/\tau_v$  as a function of wavelength  $\lambda$  in  $\text{\AA}$ . (b) Values of  $\omega_\lambda$  as a function of wavelength  $\lambda$  in  $\text{\AA}$ . (c) Values of  $g_\lambda$  for three models 1, 2, and 3. (d) Values of the unattenuated interstellar radiation field intensity  $I_0(\lambda)$ .

where  $A_m$  and  $k_m$  are constants and  $M$  is an integer such that the solution becomes exact in the limit  $M \rightarrow \infty$ . We chose  $M$  large enough to guarantee an error of less than 5% in  $J_\lambda$  at all wavelengths and optical depths. The  $M$  constants  $A_m$  are determined by the boundary conditions of equation (2). The  $M$  positive eigenvalues  $k_m$  can be written in the form

$$k_m = s_m x_\lambda, \quad (9)$$

where the  $s_m$  depend on  $\omega_\lambda$  and  $g_\lambda$ .

The solution for  $J_\lambda(\tau_v)$  contains several interesting features (Flannery, Roberge, and Rybicki 1980). The growing and decaying terms reflect contributions from the two sides of the slab, both of which contribute to the central mean intensity. Deep in optically thick clouds, the solution is dominated by the term associated with

the smallest eigenvalue,  $k_1$ , so that  $J_\lambda \sim (\exp(-k_1 \tau_v))$ . However, in optically thin clouds, such as the diffuse clouds under consideration, the solution contains significant contributions from the terms associated with several eigenvalues and from both boundaries. Both growing and decaying modes are important, and inside diffuse clouds the variation of mean intensity cannot be represented accurately by a single decaying exponential.

### III. PHOTOIONIZATION OF ATOMS AND IONS

A constituent  $i$  with photoionization cross section  $\sigma_i(\lambda)$  at wavelength  $\lambda$  is photoionized at a rate

$$\Gamma_i(\tau_v) = \frac{4\pi}{hc} \int_{\lambda_H}^{\lambda_i} \lambda \sigma_i(\lambda) J_\lambda(\tau_v) d\lambda \text{ s}^{-1}, \quad (10)$$

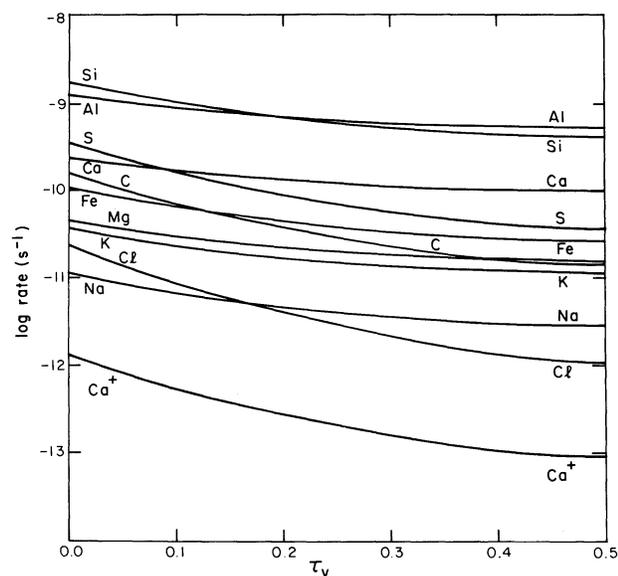


FIG. 2a

FIG. 2.—(a), (b), (c) Photoionization rates  $\Gamma_i(\tau_v)$  for models 1, 2, and 3, respectively.

TABLE 1  
SOURCES OF CROSS SECTION DATA

System	References
C	Taylor and Burke 1976; Hofmann and Trefitz 1980
Na	Hudson and Carter 1967, 1968; Chang and Kelly 1975; Amusia <i>et al.</i> 1977
Mg	Bates and Altick 1973; Dubau and Wells 1973; Amusia <i>et al.</i> 1977
Al	Chapman and Henry 1972
Si	Chapman and Henry 1972
S	Chapman and Henry 1971; Tondello 1972
Ca	Carter, Hudson, and Breig 1971; McIlrath and Sandeman 1972
Ca <sup>+</sup>	Black, Weisheit, and Laviana 1972
Fe	Kelly 1972
Cl	Brown, Carter, and Kelly 1978; Manson <i>et al.</i> 1979; Brown, Carter, and Kelly 1980
K	Hudson and Carter 1965

where the integral extends from the Lyman limit  $\lambda_H$  to the ionization threshold  $\lambda_r$ . The photoionization rates have been calculated for the systems C, Na, Mg, Al, Si, S, Fe, K, Cl, Ca, and Ca<sup>+</sup>, using cross sections taken from the references listed in Table 1.

The results are summarized in Figures 2a, 2b, and 2c for the three different grain models in a cloud with  $T_v = 0.5$ .

Comparisons of the three models is presented in Figure 3 for magnesium, Figure 4 for sulphur, and Figure 5 for chlorine. The figures contain also the photoionization rates for clouds with  $T_v = 0.3$ . Differences between the consequences of the three grain scattering models are generally larger for systems with ionization thresholds at short wavelengths and can reach an order of magnitude even in tenuous clouds of optical depths less than unity.

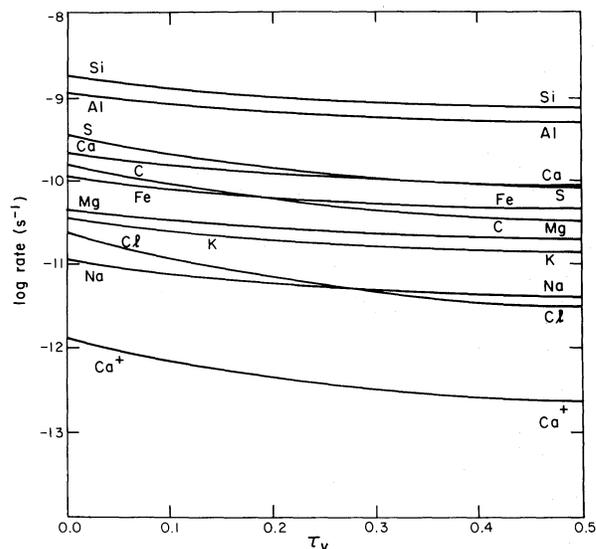


FIG. 2b

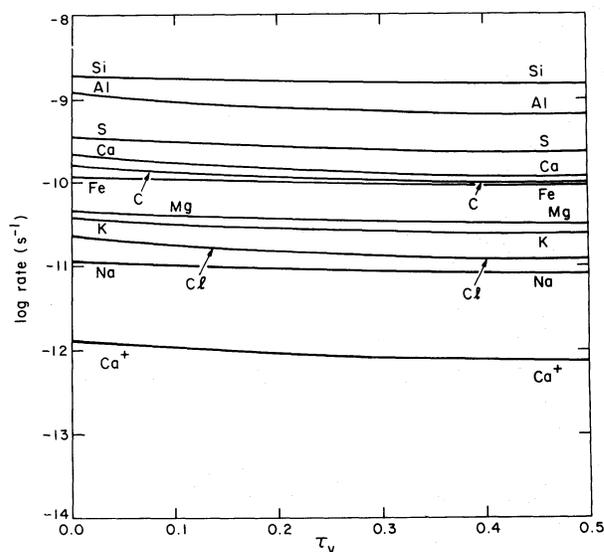


FIG. 2c

The influences of the boundaries and nonabsorptive scattering are evident. Penetration of photons through the cloud from one surface to the other is a significant effect and the photoionization rates do not depend only on  $\tau_v$  but also on the cloud size. Representations of the absorptions by exponential functions of  $\tau_v$  of the kind constructed by Black and Dalgarno (1977), though convenient, are valid only for restricted ranges of optical depths and cloud sizes.

Jenkins and Shaya (1979) have attempted to infer the characteristics of the grains by a study of the relationships between the abundances of neutral carbon, sodium, and

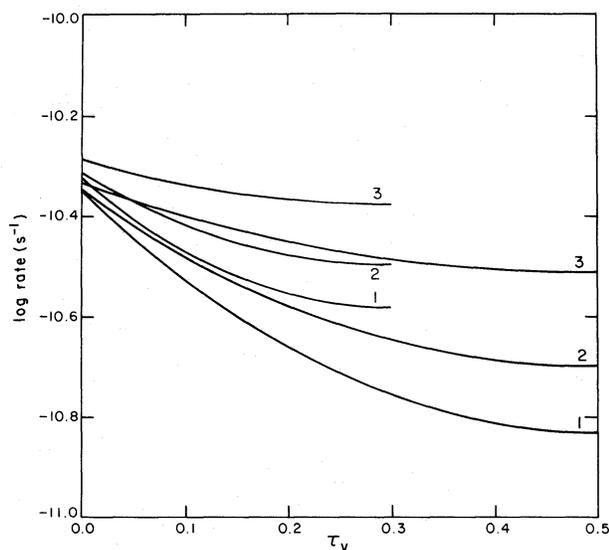


FIG. 3

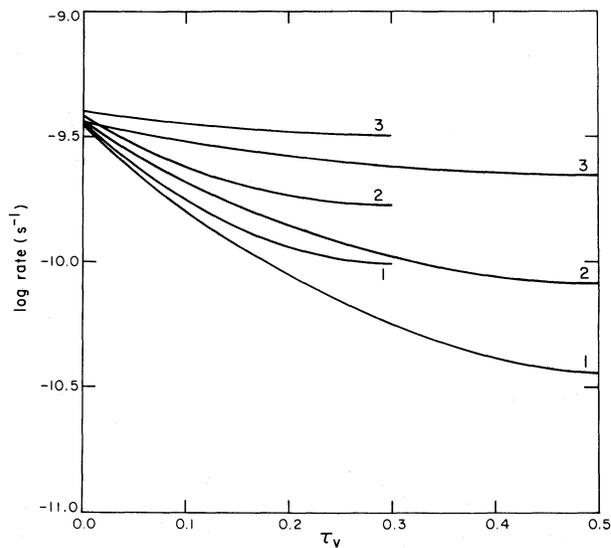


FIG. 4

FIG. 3.—Photoionization rates  $\Gamma_i(\tau_v)$  of Mg for models 1, 2, and 3 with  $T_v = 0.3$  and 0.5.FIG. 4.—Photoionization rates  $\Gamma_i(\tau_v)$  of S for models 1, 2, and 3 with  $T_v = 0.3$  and 0.5.

potassium measured toward many stars. In equilibrium between photoionization and radiative recombination, the density  $n_i$  of constituent  $i$  is related to the density  $n_i^+$  of the daughter ion by the equation

$$n_i \Gamma_i = n_i^+ \alpha_i n_e \quad (11)$$

where  $\alpha_i$  is the coefficient of radiative recombination. If  $A_i$  is the abundance of  $i$  relative to hydrogen, then the

relative abundances of two neutral components  $i = 1$  and 2 is given by

$$\frac{N_1}{N_2} = \frac{\alpha_1 A_1 \langle \Gamma_1^{-1} \rangle}{\alpha_2 A_2 \langle \Gamma_2^{-1} \rangle} \quad (12)$$

where  $\langle - \rangle$  is an average over the cloud. Equation (12) is insensitive to temperature, density, and intensity variations. Using equation (12) to interpret the observational

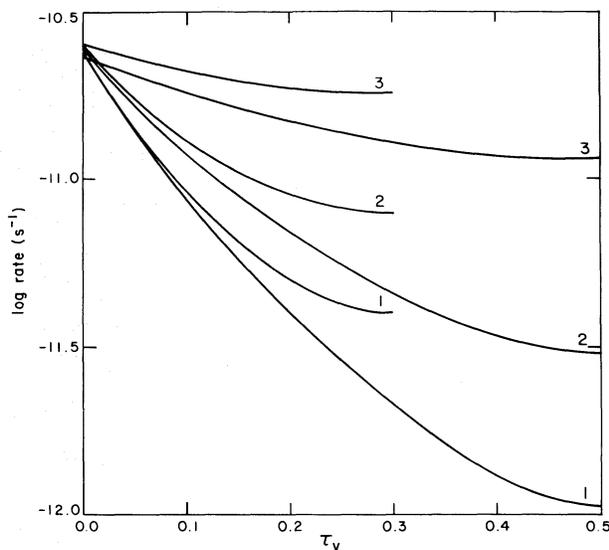


FIG. 5

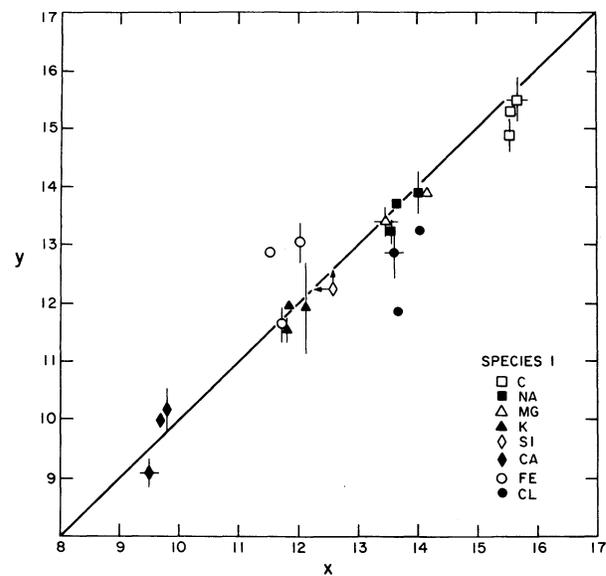


FIG. 6

FIG. 5.—Photoionization rates  $\Gamma_i(\tau_v)$  of Cl for models 1, 2, and 3 with  $T_v = 0.3$  and 0.5.FIG. 6.—The parameter  $x$  (eq. [13]) is shown as a function of  $y$  (eq. [14]).

data on C I in comparison to Na I and K I, Jenkins and Shaya (1979) concluded that the grain scattering is similar to that depicted in model 1. Because of H<sub>2</sub> line absorption, C I may not be a reliable base of comparison. We illustrate in Figure 6 a plot of the ratios for all the measured systems based on S I. In Figure 6, the coordinates are (x, y) where

$$x = \log N_i \quad (13)$$

and

$$y = \log N_s + \log \frac{\alpha_i}{\alpha_s} + \log \frac{A_i}{A_s} + \log \frac{\langle \Gamma_i^{-1} \rangle}{\langle \Gamma_s^{-1} \rangle}, \quad (14)$$

the ratio  $\langle \Gamma_i^{-1} \rangle / \langle \Gamma_s^{-1} \rangle$  being calculated from the anisotropic scattering model 3. The abundances are taken from the measurements of Morton (1975) and Snow (1976, 1977).

Agreement is excellent with the possible exception of C I, Cl I and Fe I. The C I and Cl I discrepancies may be due to the neglect of H<sub>2</sub> line absorption or to errors in the assumed radiation field intensity near the Lyman limit. The Fe I discrepancy arises from a single point. Figure 6 demonstrates that the interstellar ionization balance is consistent with a grain scattering model which is highly anisotropic for  $\lambda < 2000 \text{ \AA}$ . However a similar measure of agreement would be obtained with less anisotropic models.

Hobbs (1974, 1976) has drawn attention to observations which suggest that the column densities of Na I and K I scale approximately as the square of the atomic hydrogen column abundance, and Tarafdar (1977) has found that the observations can be represented by functions of the form

$$N(\text{Na I, K I}) \propto \{\exp(QT_v) - 1\} \quad (15)$$

which is the form expected if the ionization rate  $\Gamma$  decays exponentially with  $\tau_v$ . The observations of Ca II do not

conform to this behavior, and Tarafdar (1977) and Jenkins and Shaya (1979) attribute the failure to the fact that in diffuse clouds calcium exists mainly in the form Ca II and not as Ca III.

Using equation (11), we have calculated the fractional abundances of Na and Na<sup>+</sup> as functions of  $T_v$  for model 3 in clouds with densities  $n_H$  of  $10^2$  and  $10^3 \text{ cm}^{-3}$ . As Figures 7a and 7b demonstrate, the neutral fraction increases with  $T_v$ , and shielding effects are apparent even for grain scattering models in which shielding is diminished by forward scattering. The curves of  $\log \{N_i / (N_i + N_i^+)\}$  for Na are nearly straight lines with identical slopes of about 0.25 so that  $N_{\text{Na}}$  is given approximately by

$$N_{\text{Na}} \propto n_e T_v \exp(0.25T_v). \quad (16)$$

Equation (16), derived using model 3, has a similar shape to that obtained by Tarafdar (1977). It suggests that  $N_{\text{Na}}$  will follow the variations in  $N_H$  with some scatter arising from differences in the volume density  $n_H$  or  $n_e$ .

Similar plots for calcium are shown in Figures 8a and 8b. For clouds with  $n_H = 10^2 \text{ cm}^{-3}$ , nearly all the calcium is in the form of Ca<sup>++</sup> and the variation of  $N_{\text{Ca}^+}$  with  $N_H$  is similar to that of  $N_{\text{Na}}$ . For denser clouds, the increased electron density leads to the recombination of Ca<sup>++</sup>, and  $N_{\text{Ca}^+}$  varies linearly with  $N_H$ . Thus fluctuations in density tend to induce a large scatter in the relationship between  $N_{\text{Ca}^+}$  and  $N_H$ , as is observed (cf. Tarafdar 1977).

#### IV. PHOTOIONIZATION AND PHOTODISSOCIATION OF MOLECULES

Several studies have been carried out of the photoionization and photodissociation of interstellar molecules in diffuse and dense clouds using elaborate descriptions of the cloud chemistry in conjunction with

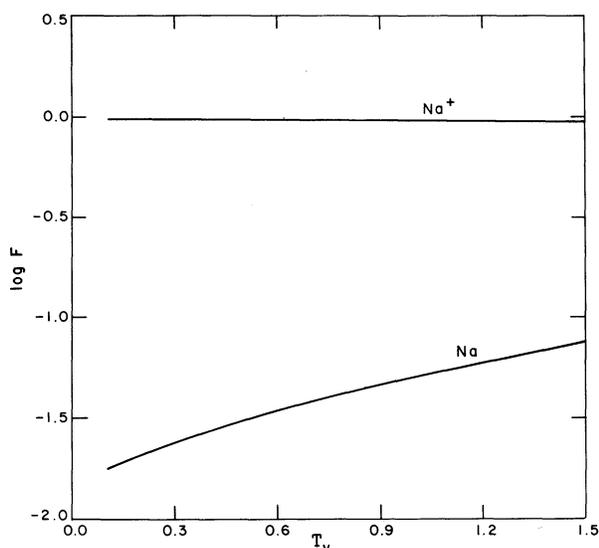


FIG. 7a

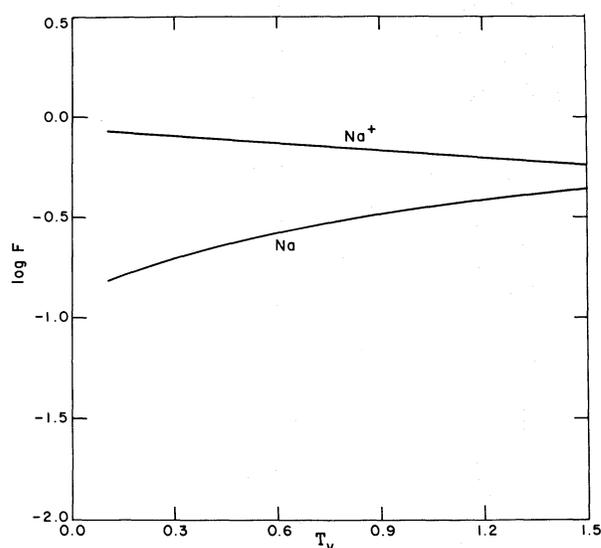


FIG. 7b

FIG. 7.—The fractional abundances  $F$  of Na and Na<sup>+</sup> as functions of  $T_v$  for (a)  $n_H = 10^2 \text{ cm}^{-3}$ , (b)  $n_H = 10^3 \text{ cm}^{-3}$ .

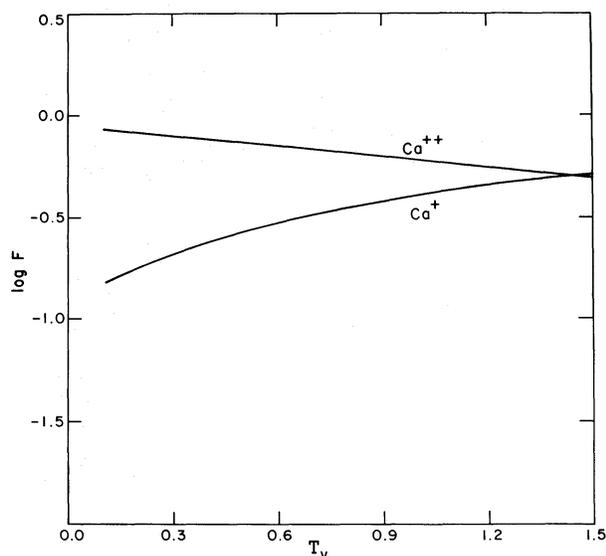


FIG. 8a

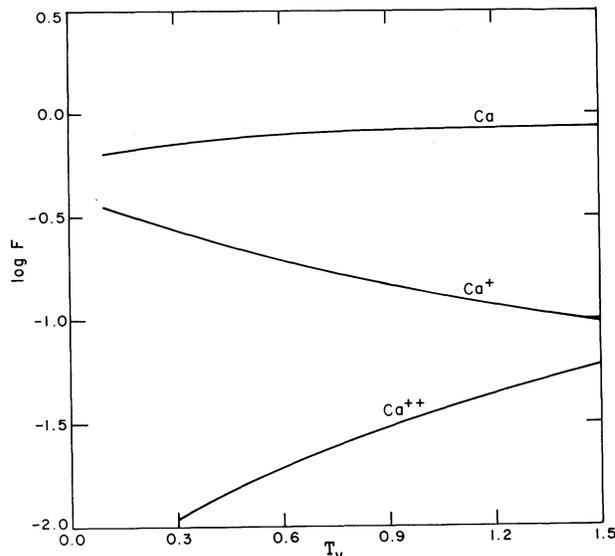


FIG. 8b

FIG. 8.—The fractional abundances  $F$  of Ca,  $\text{Ca}^+$ , and  $\text{Ca}^{++}$  as functions of  $T_v$  for (a)  $n_{\text{H}} = 10^2 \text{ cm}^{-3}$ , (b)  $n_{\text{H}} = 10^3 \text{ cm}^{-3}$ .

approximate treatments of radiative transfer (cf. Sandell 1978; Viala, Bel, and Clavel 1979; de Jong, Dalgarno, and Boland 1980), and attention has been drawn to the importance of the anisotropy in the grain scattering phase function (Sandell and Mattila 1975; Bernes and Sandqvist 1977; Sandell 1978; Clavel, Viala, and Bel 1978; Viala, Bel, and Clavel 1979).

We present here detailed calculations of photoionization rates and photodissociation rates of the interstellar molecules  $\text{CH}^+$ ,  $\text{CH}$ ,  $\text{OH}$ ,  $\text{CO}$ ,  $\text{HCl}$ ,  $\text{H}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{H}_2\text{CO}$ , and  $\text{CH}_4$  in diffuse clouds for which we have solved the radiative transfer problem with high accuracy. The sources of the cross section data are listed in Table 2.

The results for the three grain scattering models are shown in Figures 9a, 9b, and 9c. They are similar to those for the photoionization of atoms though, because the photodissociation thresholds tend to be at longer wavelengths, the differences between the scattering models are less severe for photodissociation than for

photoionization. The differences between the models are significant even for diffuse clouds and will be substantial for dense clouds.

The differences appear more clearly in Figures 10, 11, 12a, 12b, and 13 which present the results for  $\text{OH}$ ,  $\text{CO}$ ,  $\text{H}_2\text{CO}$ , and  $\text{HCl}$ . For the forward scattering model the photodestruction rates diminish slowly with increasing optical depth. If the grains scatter preferentially in the forward direction, photon induced processes remain important in the chemistry at considerable depths into

TABLE 2  
MOLECULAR CROSS SECTION DATA

Molecule	References
$\text{CH}^+$	Uzer and Dalgarno 1978; Kirby <i>et al.</i> 1980
$\text{CO}$	Solomon and Klemperer 1972
$\text{OH}$	Smith and Stella 1975
$\text{CH}$	Barsuhn and Nesbet 1978
$\text{HCl}$	Inn 1975
$\text{H}_2\text{O}$	Lee <i>et al.</i> 1978; Katayama, Huffman, and O'Bryan 1973; Ishiguro <i>et al.</i> 1978; Tan <i>et al.</i> 1978
$\text{NH}_3$	Okabe and Lenzi 1967; de Reilhac and Damany 1970; Wight, van der Wiel, and Brion 1977
$\text{H}_2\text{CO}$	Langhoff <i>et al.</i> 1978
$\text{CH}_4$	Hudson 1971; Mount, Warden, and Moos 1977; Mount and Moos 1978

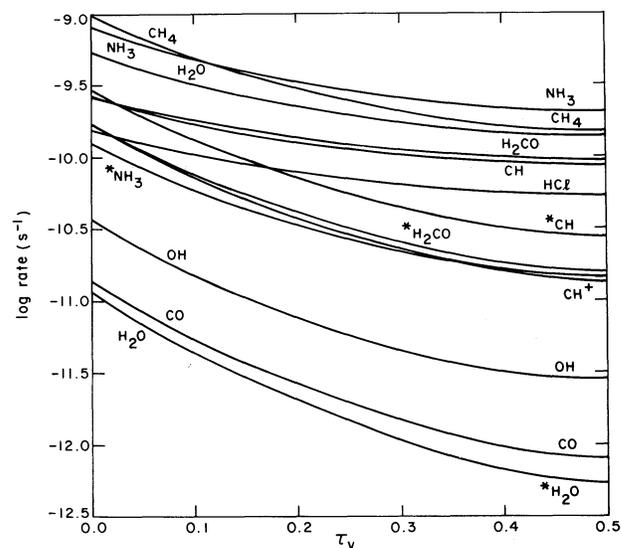


FIG. 9a

FIG. 9.—(a), (b), (c) Photodissociation and photoionization rates for models 1, 2, and 3, respectively. The asterisk denotes photoionization.

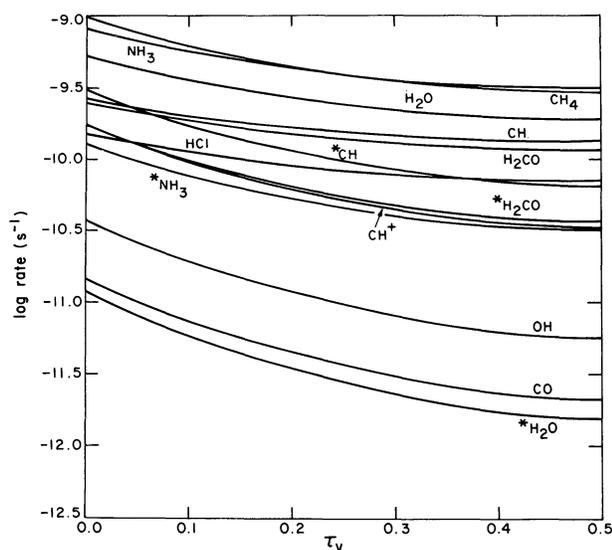


FIG. 9b

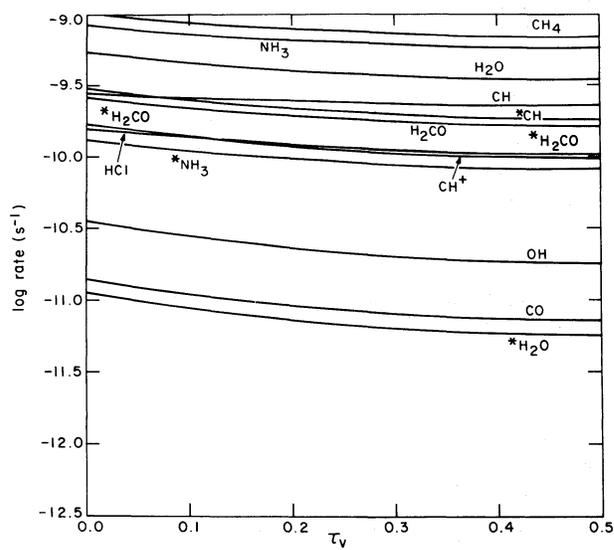


FIG. 9c

the clouds. The figures show that an exponential representation of the transmission of radiation is useful only over limited ranges.

Black and Dalgarno (1977) and Black, Hartquist, and Dalgarno (1978) have been able to construct models of the clouds towards  $\zeta$  Ophiuchi and  $\zeta$  Persei that reproduce the abundances of most of the observed interstellar molecules. Their approximate treatment of radiative transfer assumed isotropic scattering. However, the uncertainties in the chemistry and in the models are such that anisotropic scattering is not excluded. Indeed, by increasing the efficiency of destruction by photodissociation, anisotropic scattering would help to resolve the

discrepancy that exists in the case of HCl. Anisotropic scattering would also augment the supply of HCl through the reaction of  $\text{Cl}^+$  with  $\text{H}_2$ , but shielding by  $\text{H}_2$  may be effective. Alternatively the reaction of  $\text{Cl}^+$  with  $\text{H}_2$  is slow at low temperatures (Black and Smith 1980). The recent observations of neutral carbon atoms in dense clouds (Phillips *et al.* 1980) may provide stronger evidence for anisotropic scattering. It appears difficult to produce the measured abundances of neutral carbon atoms except by photodissociation of molecules such as CO,  $\text{C}_2$ , and CH. Accurate photodissociation cross section data would permit useful conclusions to be drawn about the grain scattering properties.

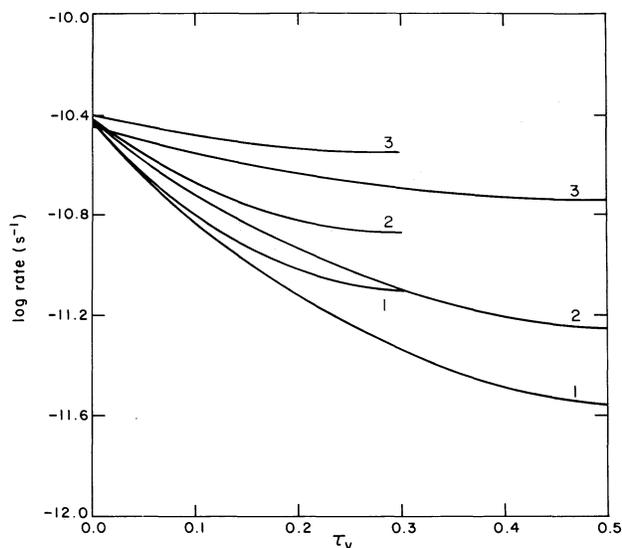


FIG. 10

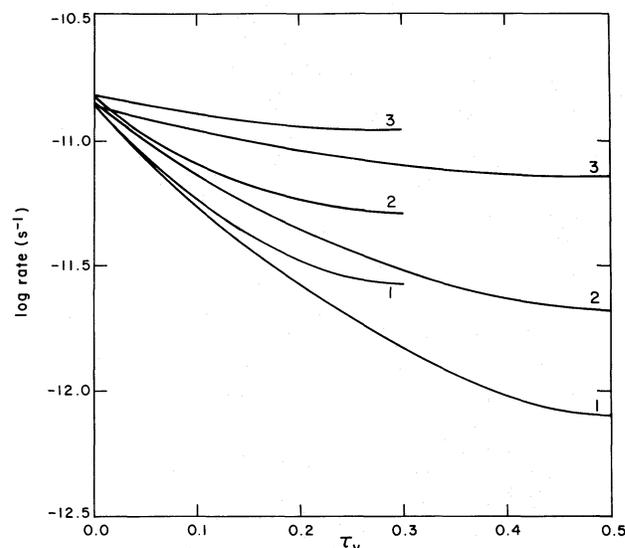


FIG. 11

FIG. 10.—Photoionization rates of OH for models 1, 2, and 3 with  $T_v = 0.3$  and 0.5.

FIG. 11.—Photoionization rates of CO for models 1, 2, and 3 with  $T_v = 0.3$  and 0.5.

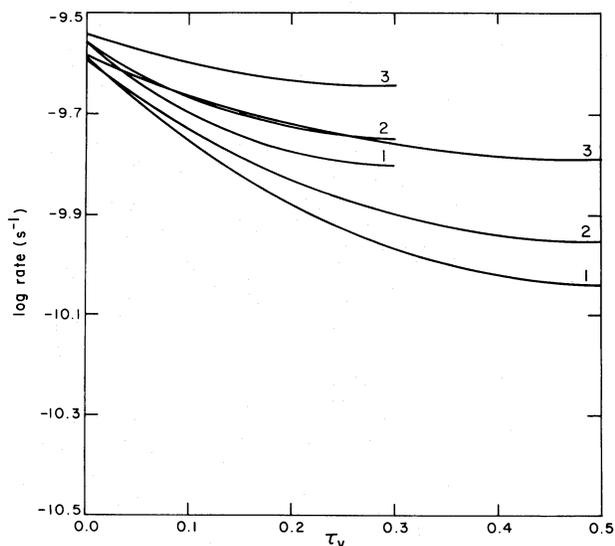


FIG. 12a

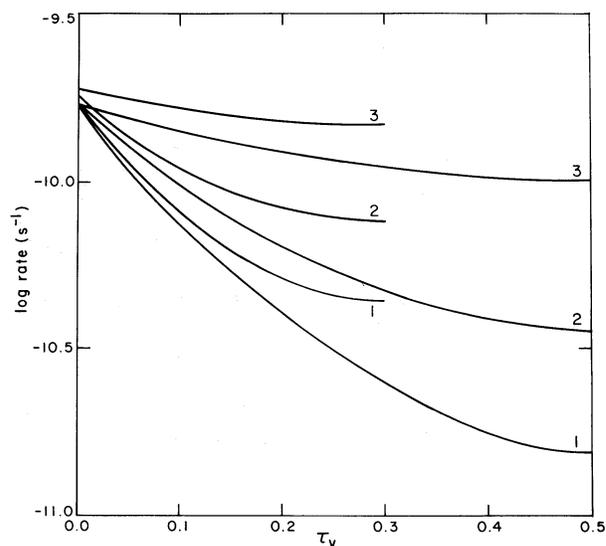


FIG. 12b

FIG. 12.—(a) Photoionization and (b) photoionization rates of  $\text{H}_2\text{CO}$  for models 1, 2, and 3 with  $T_v = 0.3$  and  $0.5$ .

## V. GRAIN HEATING

Photoelectric emission from grains is a major source of heating in diffuse clouds (cf. de Jong 1977; Draine 1978). It is strongly influenced by the scattering properties of the grains.

We used the formalism of Draine (1978) to carry out an illustrative calculation of the effects of different grain properties on the heating of an arbitrary cloud with a temperature of 100 K, a neutral hydrogen density of  $10^2 \text{ cm}^{-3}$ , a proton density of  $10^{-4} \text{ cm}^{-3}$ , and an electron

density of  $0.5 \text{ cm}^{-3}$ . The results are sensitive only to the electron density.

Photoelectrons are produced by photons with energies between some threshold  $h\nu_i$  and the Lyman limit  $h\nu_m = 13.6 \text{ eV}$ . If the grain potential is  $U$ ,  $h\nu_i = B$ , if  $U < 0$  and  $h\nu_i = eU + B$ , if  $U > 0$ , where  $B$  is a characteristic parameter of the grains. The photoelectric yield  $Y_\nu$  corresponding to a photon of frequency  $\nu$  may be represented by

$$Y_\nu = 0.5(1 - B/h\nu). \quad (17)$$

We adopt a value for  $B$  of 8 eV.

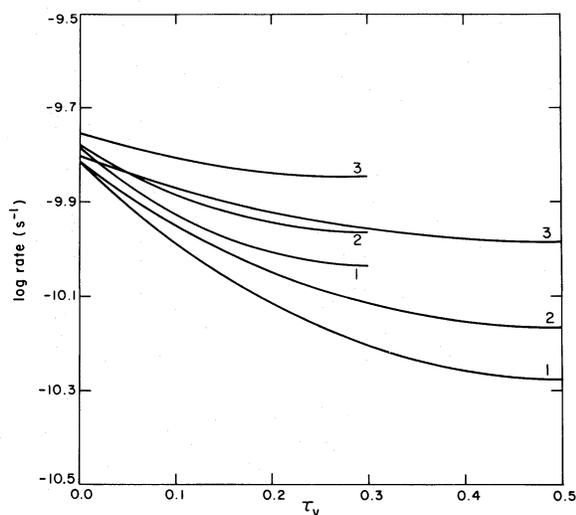


FIG. 13

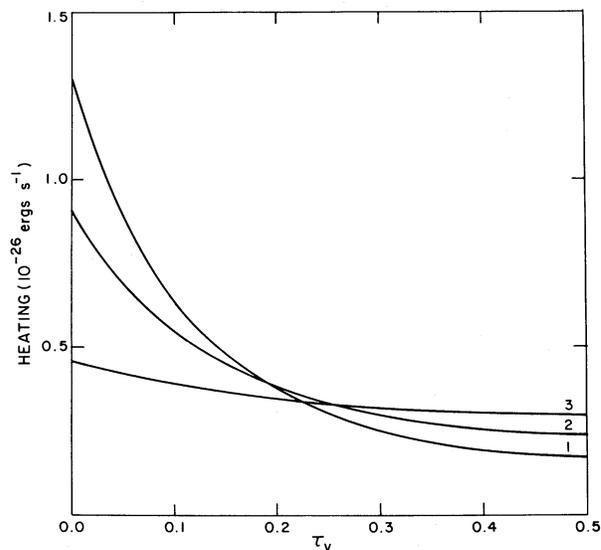


FIG. 14

FIG. 13.—Photoionization rates of  $\text{HCl}$  for models 1, 2, and 3 with  $T_v = 0.3$  and  $0.5$ .  
 FIG. 14.—Photoelectric heating rates in  $\text{ergs s}^{-1}$  per hydrogen nucleus for models 1, 2, and 3.

The photoelectric current emitted by unit area of the grain surface is given by

$$J_p(\tau_\nu) = 1.5 \int_{\nu_t}^{\nu_m} Q_\nu (1 - \omega_\nu) \frac{\pi J_\nu(\tau_\nu)}{h\nu} Y_\nu d\nu, \quad (18)$$

where  $\omega_\nu$  is the albedo at frequency  $\nu$  and  $Q_\nu$  is the ratio of the grain extinction cross section to the geometrical cross section. The threshold frequency  $\nu_t$  depends upon the grain potential  $U$  which may be obtained from the condition that the photoelectric current is balanced by the rate at which the protons and electrons adhere to the grains. According to Draine (1978), the protons adhere with a sticking factor of unity, and the electrons adhere with a sticking factor of 0.5.

The net heating rate is expressible in terms of  $\phi = eU/kT$ , an accommodation coefficient  $\alpha_H$  for atomic

hydrogen, and a grain geometric cross section  $\sigma$ . Following Draine (1978), we adopt  $\alpha_H = 0.14$  and  $\sigma = 1.5 \times 10^{-21} \text{ cm}^2$ .

The resulting rates of heat deposition for our three models of the grain scattering are presented in Figure 14. At small optical depths, heating is greatest for the isotropic scattering model for which the albedo  $\omega_\nu$  is small; but at large optical depths, forward scattering substantially enhances the heating, and heating is greatest for anisotropic scattering. Indeed the heat deposition occurring in the forward scattering case varies little with optical depth in diffuse clouds.

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