

INTERSTELLAR PHOTODISSOCIATION AND PHOTOIONIZATION RATES

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ABSTRACT

The rates of photoionization and photodissociation of molecules are calculated as functions of visual extinction into plane-parallel clouds illuminated by the average interstellar radiation field. An accurate technique is used to calculate the attenuation of the ultraviolet radiation due to scattering and absorption by dust grains inside the clouds. As a plausible and self-consistent model for the grains in diffuse clouds and the outer layers of dense clouds, the graphite-silicate grain mixture of Mathis, Rumpl, & Nordsieck is adopted, together with the wavelength-dependent grain optical properties calculated by Draine & Lee. Depth-dependent photodissociation and photoionization rates are presented for a wide range of molecules, and the results are compared with the rates of photodestruction resulting from internal photons generated by cosmic rays.

Subject headings: interstellar: grains — interstellar: molecules — molecular processes

1. INTRODUCTION

Interstellar radiation leads to the photodissociation and photoionization of molecular species in interstellar clouds and the envelopes of dense clouds. Photon-induced processes are particularly important in so-called photodissociation (Hollenbach 1988 and references therein), photochemical (van Dishoeck 1988a), or photon-dominated regions, which are cloud components subjected to intense radiation from nearby or embedded stars.

The radiation field inside the clouds is attenuated by the absorption and scattering of photons due to dust particles present in the gas. The influence of dust on the photodestruction rates of interstellar molecules has been explored by Sandell & Mattila (1975), Whitworth (1975), Bernes & Sandqvist (1977), Sandell (1978), van Dishoeck & Dalgarno (1984), and Aiello et al. (1987). Roberge, Dalgarno, & Flannery (1981) used the accurate "spherical harmonics method" (Flannery, Roberge, & Rybicki 1980) to solve the equation of radiative transfer for diffuse, plane-parallel clouds illuminated on both sides by the average interstellar radiation field (ISRF). Similar calculations for clouds of greater column density were carried out by van Dishoeck (1987, 1988b). The calculations described below extend the previous work on this problem by calculating the photodestruction rates of some species not considered elsewhere, and by adopting a more realistic model for the grain scattering and absorption cross sections.

2. CALCULATIONS

A photodestruction process i , with cross section $\sigma_i(\lambda)$, proceeds at a rate

$$\Gamma_i(A_v) = 4\pi \int_{\lambda_H}^{\lambda_i} J_\lambda(A_v) \sigma_i(\lambda) d\lambda, \quad (1)$$

where Γ_i depends on the extinction A_v in visual magnitudes measured inward from the cloud surface, $J_\lambda(A_v)$ is the mean intensity of radiation at depth A_v in photons $\text{cm}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{nm}^{-1}$, and the integral over wavelength runs from $\lambda_H = 91.2$ nm to the threshold wavelength λ_i for the process of interest. We have used the spherical harmonics method to solve the equation of radiative transfer for $J_\lambda(A_v)$ as a function of λ and A_v for three exemplary clouds with total visual extinctions $A_v^{\text{tot}} = 1, 10, \text{ and } 100$ mag. The relevant transfer equation and solution method are described in detail elsewhere (Flannery et al. 1980). The boundary conditions and other information required to determine uniquely the radiation field were chosen as follows.

The clouds were assumed to be illuminated isotropically at both surfaces by the average interstellar radiation field with specific intensity

$$I_\lambda = 2.549 \times 10^{12} \left(\frac{\lambda}{\text{nm}} \right)^{-3} - 4.102 \times 10^{14} \left(\frac{\lambda}{\text{nm}} \right)^{-4} + 1.635 \times 10^{16} \left(\frac{\lambda}{\text{nm}} \right)^{-5} \quad (2)$$

photons $\text{cm}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{nm}^{-1}$ at wavelengths $\lambda < 240$ nm (Draine 1978). At longer wavelengths, I_λ was approximated by a dilute blackbody spectrum with a temperature of 10^4 K and a dilution factor chosen to make I_λ continuous at $\lambda = 240$ nm.

As a preliminary step in the evaluation of the photodestruction rates (1), we found $J_\lambda(A_v)$ by solving the transfer equation on a grid of λ values. At each wavelength we needed A_λ/A_v , the ratio of grain extinction cross sections at λ and $\lambda_v = 550$ nm, as well as the grain albedo ω_λ and the "asymmetry factor" g_λ , which parameterizes the Henyey-Greenstein grain scattering phase function. Previous calculations by us (Roberge et al. 1981) and by others using our radiative transfer codes (van

Dishoeck & Dalgarno 1984; van Dishoeck 1986, 1988b) employed three empirical models of the grain properties. In these models, the grain properties were inferred from observations of the diffuse interstellar medium, with ad hoc extrapolation at wavelengths where the observational data were unavailable. In particular, it was necessary to extrapolate A_λ/A_V for $\lambda < 100$ nm and the scattering properties ω_λ and g_λ for $\lambda < 155$ nm. However ad hoc extrapolations of this sort are subject to two types of error: First, the scattering properties of grains in the far-ultraviolet are strongly constrained by observations at longer wavelengths, independent of assumptions about grain size and composition (Chlewicki & Greenberg 1984). Among the grain models considered by Roberge et al. (1981), only their model 2 satisfies these constraints. Second, ad hoc extrapolations produce grain properties descriptive of fictitious grains whose dielectric function will, in general, fail to satisfy the Kramers-Kronig dispersion relation (e.g., Jackson 1975).

In this paper we adopt the more realistic set of grain properties calculated by Draine & Lee (1984) and shown in Figures 1 and 2. The calculations of Draine & Lee describe the "Mathis-Rumpl-Nordsieck" mixture of graphite and silicate grains with a power-law distribution of radii (Mathis, Rumpl, & Nordsieck 1977). While the exact composition of grains is a controversial subject (see the review of Mathis 1986), the MRN model reproduces the average extinction curve for the diffuse interstellar medium. Further, the Draine-Lee model makes ex-

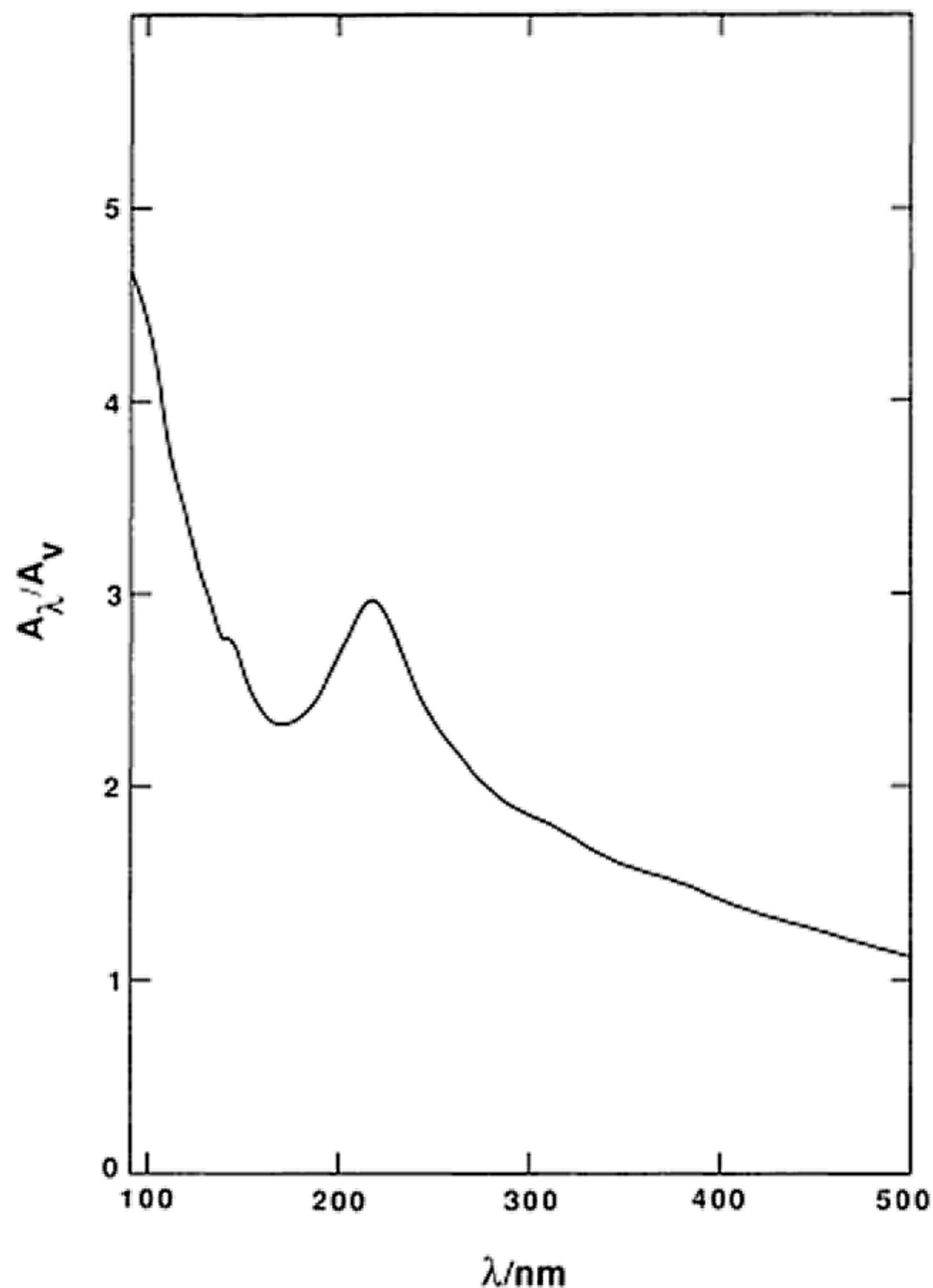


FIG. 1.—Extinction A_λ at wavelength λ relative to the extinction A_V at $\lambda = 550$ nm for the grain model adopted here (see text).

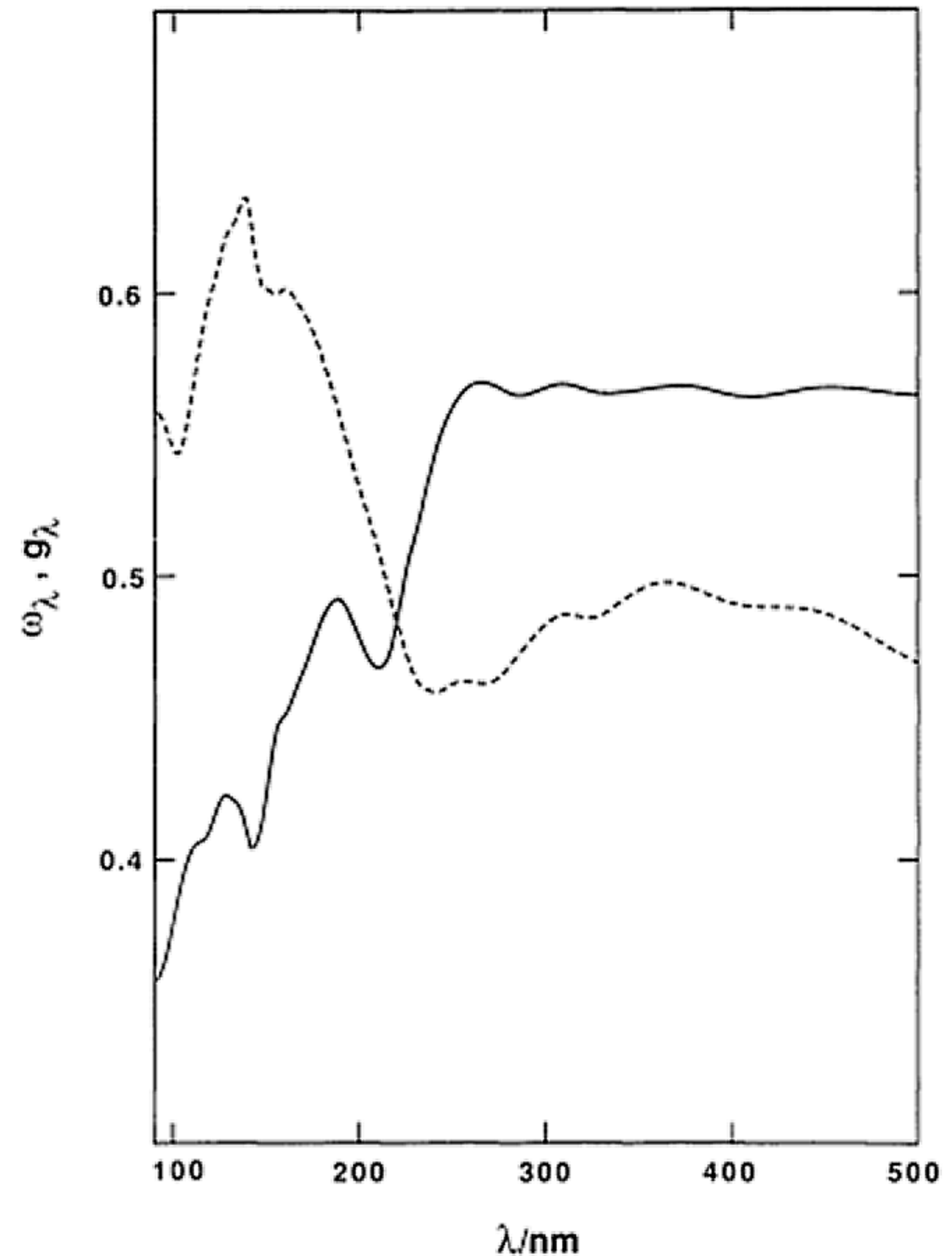


FIG. 2.—The single-scattering albedo ω_λ (solid curve) and Henyey-Greenstein asymmetry factor g_λ (dashed curve) for the grain model adopted here.

tensive use of laboratory data on the dielectric properties of graphite and silicates, is consistent with model-independent constraints on grain scattering properties (Chlewicki & Greenberg 1984), and obeys the Kramers-Kronig relation. For an illustrative example of alternative grain models and their effects on calculations of the UV radiation field inside clouds, see Roberge (1990, Fig. 2).

Finally, we caution the reader that significant fluctuations exist in the optical properties of grains along different lines of sight, especially at the far-ultraviolet wavelengths of interest here (Massa & Savage 1989, and references therein). The fluctuations, which correlate strongly with R , the ratio of total-to-selective extinction (Cardelli, Clayton, & Mathis 1989), have important chemical consequences, even in diffuse clouds (Cardelli 1988). Our results apply strictly to the "average cloud" in a region of the diffuse interstellar medium where $R = 3.1$.

3. PHOTODISSOCIATION AND PHOTOIONIZATION RATES

The unattenuated photodissociation and photoionization rates corresponding to the average interstellar radiation field (Draine 1978, eq. [2]) are given in Table 1 where they are compared with values calculated by Herbst & Leung (1986) and van Dishoeck (1987, 1988b). The cross sections are often uncertain, and where discrepancies arise they can be attributed

TABLE 1
PHOTODISSOCIATION AND PHOTOIONIZATION RATES (s^{-1})
FOR AN UNATTENUATED RADIATION FIELD

reaction	this work	van Dishoeck (1988)	Herbst and Leung (1986)
$NO_2 \rightarrow NO + O$	1.2(-09)	1.4(-09)	
$SO_2 \rightarrow SO + O$	1.9(-09)	1.9(-09)	2.1(-09)
$CS_2 \rightarrow CS + S$	6.9(-09)	6.1(-09)	
$OCS \rightarrow CO + S$	3.7(-09)	3.7(-09)	4.6(-09)
$OCS \rightarrow OCS^+ + e$	4.2(-10)	7.0(-10)	4.7(-10)
$NH_3 \rightarrow NH_2 + H$	1.1(-09)	1.1(-09)	9.9(-10)
$NH_3 \rightarrow NH_3^+ + e$	1.8(-10)	2.8(-10)	2.4(-10)
$CH_4 \rightarrow CH_2 + H_2$	9.8(-10)	1.2(-09)	
$H_2O_2 \rightarrow 2OH$	8.3(-10)	9.4(-10)	
$C_2H_2 \rightarrow C_2H + H$	7.3(-09)	3.2(-09)	3.6(-09)
$C_2H_2 \rightarrow C_2H_2^+ + e$	4.6(-10)	3.3(-09)	4.1(-10)
$H_2CO \rightarrow H_2 + CO$	1.4(-09)	1.0(-09)	
$CH_3OH \rightarrow CH_3 + OH$	1.2(-09)	1.4(-09)	
$CH_3OH \rightarrow CH_3O^+ + H + e$	9.3(-12)		
$CH_3OH \rightarrow CH_3O^+ + e$	7.0(-10)		
$C_2 \rightarrow C + C$	1.5(-10)	2.3(-10)	9.4(-11)
$CH^+ \rightarrow C + H^+$	2.5(-10)	3.2(-10)	
$NH_2 \rightarrow NH + H$	3.9(-10)	7.4(-10)	4.2(-10)
$CO_2 \rightarrow CO + O$	1.4(-09)	8.7(-10)	6.2(-10)
$O_2 \rightarrow O + O$	6.9(-10)	7.9(-10)	
$O_2 \rightarrow O_2^+ + e$	5.6(-11)	7.7(-11)	
$CH \rightarrow C + H$	8.6(-10)	9.5(-10)	
$HCl \rightarrow H + Cl$	1.1(-09)	9.8(-10)	
$C_4H_2 \rightarrow C_4H + H$	1.9(-09)		2.2(-09)
$C_4H_2 \rightarrow C_4H_2^+ + e$	4.6(-10)		5.2(-10)
$C_4H_2 \rightarrow C_2H + C_2H$	1.9(-09)		2.2(-09)
$NO \rightarrow N + O$	4.3(-10)	4.7(-10)	
$H_2O \rightarrow H + OH$	5.9(-10)	6.7(-10)	6.6(-10)
$HCN \rightarrow H + CN$	1.3(-09)	1.5(-09)	1.1(-09)
$C_3 \rightarrow C_2 + C$	3.8(-09)	3.8(-09)	5.2(-09)
$CH_5N \rightarrow HCN + H_2 + 2H$	8.6(-10)		7.0(-10)
$CH_5N \rightarrow CH_3N + 2H$	8.7(-11)		1.3(-10)
$CH_5N \rightarrow CH_3 + NH_2$	4.0(-10)		3.1(-10)
$CH_5N \rightarrow CN + 2H_2 + H$	2.2(-10)		1.9(-10)
$CH_5N \rightarrow CH_5N^+ + e$	4.6(-10)		5.2(-10)
$CH_3N \rightarrow HCN + H_2$	3.5(-09)		3.4(-09)
$CH_3OCH_3 \rightarrow H_2CO + CH_4$	1.5(-09)		1.6(-09)
$CH_3OCH_3 \rightarrow CH_3OCH_3^+ + e$	4.6(-10)		5.2(-10)
$HC_3N \rightarrow C_2H + CN$	7.4(-09)	5.6(-09)	3.4(-09)
$C_2H_4 \rightarrow C_2H_2 + H_2$	3.0(-09)	3.0(-09)	3.2(-09)
$C_2H_4 \rightarrow C_2H_4^+ + e$	2.6(-10)	4.1(-10)	2.4(-10)
$CH_2O_2 \rightarrow HCO + OH$	4.1(-10)		5.5(-10)
$CH_2O_2 \rightarrow CH_2O_2^+ + e$	2.6(-10)		3.5(-10)
$C_2H_2O \rightarrow CH_2 + CO$	1.4(-09)		1.8(-09)
$C_2H_2O \rightarrow C_2H_2O^+ + e$	6.6(-10)		6.9(-10)
$C_2H_3N \rightarrow CH_3 + CN$	3.4(-09)	2.4(-09)	3.1(-09)
$C_2H_3N \rightarrow C_2H_3N^+ + e$	6.2(-10)		1.1(-09)
$C_2H_3OH \rightarrow C_2H_3 + OH$	2.9(-09)		2.8(-09)
$C_2H_3OH \rightarrow C_2H_3OH^+ + e$	1.0(-09)		1.1(-09)
$C_2H_4O \rightarrow CH_3 + HCO$	1.1(-09)		6.9(-10)
$C_2H_4O \rightarrow CH_4 + CO$	1.1(-09)		6.9(-10)
$C_2H_4O \rightarrow C_2H_4O^+ + e$	4.6(-10)		5.2(-10)
$C_3O \rightarrow C_2 + CO$	7.0(-09)		9.0(-09)
$CN \rightarrow C + N$	1.1(-09)	3.0(-10)	2.0(-9)
$HCO \rightarrow HCO^+ + e$	5.6(-10)		4.9(-10)
$HNCO \rightarrow NH + CO$	1.8(-09)		
$C_3H_4 \rightarrow C_3H_3 + H$	3.3(-09)		3.7(-09)
$C_3H_4 \rightarrow C_3H_4^+ + e$	2.2(-09)		2.0(-09)
$H_2S \rightarrow H_2 + S$	2.9(-09)	3.1(-09)	
$H_2S \rightarrow H_2S^+ + e$	6.3(-10)	7.1(-10)	
$OH \rightarrow O + H$	3.5(-10)	4.2(-10)	3.4(-10)

TABLE 2A
 PHOTODISSOCIATION AND PHOTOIONIZATION RATES (s^{-1}) VERSUS A_v FOR A CLOUD WITH $A_v^{tot} = 1$

reaction	$A_v/$	0.0	0.1	0.2	0.3	0.4	0.5
$NO_2 \rightarrow NO + O$		7.00(-10)	4.60(-10)	3.54(-10)	2.96(-10)	2.65(-10)	2.56(-10)
$SO_2 \rightarrow SO + O$		1.05(-09)	6.56(-10)	4.89(-10)	3.97(-10)	3.49(-10)	3.34(-10)
$CS_2 \rightarrow CS + S$		4.00(-09)	2.68(-09)	2.10(-09)	1.77(-09)	1.60(-09)	1.54(-09)
$OCS \rightarrow CO + S$		2.12(-09)	1.42(-09)	1.10(-09)	9.31(-10)	8.40(-10)	8.11(-10)
$OCS \rightarrow OCS^+ + e$		2.30(-10)	1.18(-10)	7.58(-11)	5.39(-11)	4.29(-11)	3.96(-11)
$NH_3 \rightarrow NH_2 + H$		6.12(-10)	3.89(-10)	2.94(-10)	2.41(-10)	2.14(-10)	2.05(-10)
$NH_3 \rightarrow NH_3^+ + e$		9.58(-11)	5.05(-11)	3.33(-11)	2.42(-11)	1.96(-11)	1.82(-11)
$CH_4 \rightarrow CH_2 + H_2$		5.45(-10)	3.26(-10)	2.35(-10)	1.86(-10)	1.60(-10)	1.52(-10)
$H_2O_2 \rightarrow 2OH$		4.69(-10)	2.95(-10)	2.22(-10)	1.81(-10)	1.60(-10)	1.53(-10)
$C_2H_2 \rightarrow C_2H + H$		4.15(-09)	2.68(-09)	2.05(-09)	1.70(-09)	1.51(-09)	1.45(-09)
$C_2H_2 \rightarrow C_2H_2^+ + e$		2.50(-10)	1.31(-10)	8.60(-11)	6.23(-11)	5.03(-11)	4.67(-11)
$H_2CO \rightarrow H_2 + CO$		8.22(-10)	5.37(-10)	4.13(-10)	3.44(-10)	3.08(-10)	2.96(-10)
$CH_3OH \rightarrow CH_3 + OH$		6.56(-10)	4.06(-10)	3.00(-10)	2.43(-10)	2.13(-10)	2.04(-10)
$CH_3OH \rightarrow CH_3O^+ + H + e$		5.03(-12)	2.52(-12)	1.59(-12)	1.12(-12)	8.77(-13)	8.04(-13)
$CH_3OH \rightarrow CH_4O + e$		3.86(-10)	2.09(-10)	1.40(-10)	1.04(-10)	8.52(-11)	7.94(-11)
$C_2 \rightarrow C + C$		8.27(-11)	4.85(-11)	3.46(-11)	2.72(-11)	2.33(-11)	2.21(-11)
$CH^+ \rightarrow C + H^+$		1.37(-10)	6.87(-11)	4.37(-11)	3.07(-11)	2.42(-11)	2.22(-11)
$NH_2 \rightarrow NH + H$		2.28(-10)	1.64(-10)	1.34(-10)	1.17(-10)	1.07(-10)	1.05(-10)
$CO_2 \rightarrow CO + O$		7.41(-10)	4.04(-10)	2.74(-10)	2.04(-10)	1.69(-10)	1.58(-10)
$O_2 \rightarrow O + O$		3.91(-10)	2.57(-10)	1.98(-10)	1.66(-10)	1.48(-10)	1.43(-10)
$O_2 \rightarrow O_2^+ + e$		3.04(-11)	1.50(-11)	9.37(-12)	6.48(-12)	5.05(-12)	4.62(-12)
$CH \rightarrow C + H$		5.05(-10)	3.54(-10)	2.85(-10)	2.46(-10)	2.25(-10)	2.19(-10)
$HCl \rightarrow H + Cl$		6.22(-10)	3.86(-10)	2.86(-10)	2.32(-10)	2.03(-10)	1.94(-10)
$C_4H_2 \rightarrow C_4H + H$		1.06(-09)	7.15(-10)	5.59(-10)	4.73(-10)	4.28(-10)	4.13(-10)
$C_4H_2 \rightarrow C_4H_2^+ + e$		2.51(-10)	1.40(-10)	9.67(-11)	7.34(-11)	6.14(-11)	5.77(-11)
$C_4H_2 \rightarrow C_2H + C_2H$		1.06(-09)	7.15(-10)	5.59(-10)	4.73(-10)	4.28(-10)	4.13(-10)
$NO \rightarrow N + O$		2.47(-10)	1.62(-10)	1.25(-10)	1.04(-10)	9.32(-11)	8.98(-11)
$H_2O \rightarrow H + OH$		3.34(-10)	2.14(-10)	1.62(-10)	1.33(-10)	1.19(-10)	1.14(-10)
$HCN \rightarrow H + CN$		7.00(-10)	4.09(-10)	2.91(-10)	2.27(-10)	1.94(-10)	1.84(-10)
$C_3 \rightarrow C_2 + C$		2.17(-09)	1.49(-09)	1.18(-09)	1.01(-09)	9.20(-10)	8.91(-10)
$CH_3N \rightarrow HCN + H_2 + 2H$		4.79(-10)	2.90(-10)	2.12(-10)	1.70(-10)	1.47(-10)	1.40(-10)
$CH_3N \rightarrow CH_3N + 2H$		5.13(-11)	3.69(-11)	3.01(-11)	2.63(-11)	2.43(-11)	2.36(-11)
$CH_3N \rightarrow CH_3 + NH_2$		2.23(-10)	1.33(-10)	9.61(-11)	7.61(-11)	6.56(-11)	6.24(-11)
$CH_3N \rightarrow CN + 2H_2 + H$		1.23(-10)	7.49(-11)	5.47(-11)	4.37(-11)	3.80(-11)	3.62(-11)
$CH_3N \rightarrow CH_3N^+ + e$		2.51(-10)	1.40(-10)	9.67(-11)	7.34(-11)	6.14(-11)	5.77(-11)
$CH_3N \rightarrow HCN + H_2$		2.00(-09)	1.29(-09)	9.83(-10)	8.16(-10)	7.28(-10)	7.00(-10)
$CH_3OCH_3 \rightarrow H_2CO + CH_4$		8.35(-10)	5.41(-10)	4.14(-10)	3.44(-10)	3.07(-10)	2.96(-10)
$CH_3OCH_3 \rightarrow CH_3OCH_3^+ + e$		2.51(-10)	1.40(-10)	9.67(-11)	7.34(-11)	6.14(-11)	5.77(-11)
$C_3HN \rightarrow C_2H + CN$		4.17(-09)	2.66(-09)	2.00(-09)	1.64(-09)	1.45(-09)	1.40(-09)
$C_2H_4 \rightarrow C_2H_2 + H_2$		1.69(-09)	1.11(-09)	8.55(-10)	7.15(-10)	6.42(-10)	6.19(-10)
$C_2H_4 \rightarrow C_2H_4^+ + e$		1.40(-10)	7.40(-11)	4.88(-11)	3.55(-11)	2.88(-11)	2.67(-11)
$CH_2O_2 \rightarrow HCO + OH$		2.33(-10)	1.50(-10)	1.14(-10)	9.43(-11)	8.38(-11)	8.05(-11)
$CH_2O_2 \rightarrow CH_2O_2^+ + e$		1.44(-10)	7.67(-11)	5.11(-11)	3.74(-11)	3.05(-11)	2.84(-11)
$C_2H_3O \rightarrow CH_2 + CO$		8.16(-10)	5.60(-10)	4.43(-10)	3.79(-10)	3.44(-10)	3.33(-10)
$C_2H_3O \rightarrow C_2H_3O^+ + e$		3.66(-10)	2.14(-10)	1.52(-10)	1.19(-10)	1.01(-10)	9.59(-11)
$C_2H_3N \rightarrow CH_3 + CN$		1.86(-09)	1.07(-09)	7.60(-10)	5.91(-10)	5.04(-10)	4.76(-10)
$C_2H_3N \rightarrow C_2H_3N^+ + e$		3.35(-10)	1.68(-10)	1.06(-10)	7.44(-11)	5.85(-11)	5.36(-11)
$C_2H_3OH \rightarrow C_2H_2 + OH$		1.61(-09)	9.87(-10)	7.27(-10)	5.85(-10)	5.12(-10)	4.89(-10)
$C_2H_3OH \rightarrow C_2H_3OH^+ + e$		5.51(-10)	2.99(-10)	2.01(-10)	1.50(-10)	1.23(-10)	1.15(-10)
$C_2H_4O \rightarrow CH_3 + CHO$		6.43(-10)	4.57(-10)	3.70(-10)	3.21(-10)	2.95(-10)	2.87(-10)
$C_2H_4O \rightarrow CH_4 + CO$		6.43(-10)	4.57(-10)	3.70(-10)	3.21(-10)	2.95(-10)	2.87(-10)
$C_2H_4O \rightarrow C_2H_4O^+ + e$		2.51(-10)	1.40(-10)	9.67(-11)	7.34(-11)	6.14(-11)	5.77(-11)
$C_3O \rightarrow C_2 + CO$		4.07(-09)	2.83(-09)	2.27(-09)	1.95(-09)	1.78(-09)	1.73(-09)
$CN \rightarrow C + N$		5.93(-10)	2.99(-10)	1.90(-10)	1.34(-10)	1.05(-10)	9.66(-11)
$HCO \rightarrow HCO^+ + e$		3.08(-10)	1.77(-10)	1.24(-10)	9.60(-11)	8.13(-11)	7.68(-11)
$HNCO \rightarrow NH + CO$		9.93(-10)	6.39(-10)	4.85(-10)	4.01(-10)	3.56(-10)	3.42(-10)
$C_3H_4 \rightarrow C_3H_3 + H$		1.86(-09)	1.20(-09)	9.11(-10)	7.53(-10)	6.69(-10)	6.43(-10)
$C_3H_4 \rightarrow C_3H_4^+ + e$		1.18(-09)	6.51(-10)	4.43(-10)	3.32(-10)	2.76(-10)	2.58(-10)
$H_2S \rightarrow H_2 + S$		1.62(-09)	9.67(-10)	6.99(-10)	5.54(-10)	4.79(-10)	4.56(-10)
$H_2S \rightarrow H_2S^+ + e$		3.44(-10)	1.81(-10)	1.20(-10)	8.73(-11)	7.08(-11)	6.57(-11)
$OH \rightarrow O + H$		1.99(-10)	1.23(-10)	9.19(-11)	7.48(-11)	6.59(-11)	6.31(-11)

TABLE 2B

PHOTODISSOCIATION AND PHOTOIONIZATION RATES (s^{-1}) VERSUS A_v FOR A CLOUD WITH $A_v^{tot} = 10$

reaction	$A_v/$	0.0	1.0	2.0	3.0	4.0	5.0
$NO_2 \rightarrow NO + O$		6.64(-10)	3.90(-11)	4.67(-12)	6.45(-13)	9.82(-14)	2.97(-14)
$SO_2 \rightarrow SO + O$		1.01(-09)	4.49(-11)	4.21(-12)	4.70(-13)	5.98(-14)	1.58(-14)
$CS_2 \rightarrow CS + S$		3.78(-09)	2.44(-10)	3.01(-11)	4.16(-12)	6.16(-13)	1.80(-13)
$OCS \rightarrow CO + S$		2.01(-09)	1.28(-10)	1.60(-11)	2.27(-12)	3.47(-13)	1.05(-13)
$OCS \rightarrow OCS^+ + e$		2.27(-10)	3.03(-12)	9.09(-14)	3.15(-15)	1.20(-16)	9.78(-18)
$NH_3 \rightarrow NH_2 + H$		5.85(-10)	2.94(-11)	3.19(-12)	4.12(-13)	5.93(-14)	1.72(-14)
$NH_3 \rightarrow NH_3^+ + e$		9.44(-11)	1.52(-12)	5.34(-14)	2.11(-15)	8.89(-17)	7.78(-18)
$CH_4 \rightarrow CH_3 + H$		5.28(-10)	1.81(-11)	1.32(-12)	1.11(-13)	1.02(-14)	1.95(-15)
$H_2O_2 \rightarrow 2OH$		4.49(-10)	2.12(-11)	2.13(-12)	2.54(-13)	3.40(-14)	9.31(-15)
$C_2H_2 \rightarrow C_2H + H$		3.95(-09)	2.10(-10)	2.19(-11)	2.57(-12)	3.27(-13)	8.34(-14)
$C_2H_2 \rightarrow C_2H_2^+ + e$		2.46(-10)	3.86(-12)	1.35(-13)	5.38(-15)	2.30(-16)	2.04(-17)
$H_2CO \rightarrow H_2 + CO$		7.81(-10)	4.43(-11)	5.04(-12)	6.59(-13)	9.48(-14)	2.74(-14)
$CH_3OH \rightarrow CH_3 + OH$		6.30(-10)	2.72(-11)	2.59(-12)	3.00(-13)	3.95(-14)	1.07(-14)
$CH_3OH \rightarrow CH_3O^+ + H + e$		4.97(-12)	5.70(-14)	1.39(-15)	3.64(-17)	9.74(-19)	5.25(-20)
$CH_3OH \rightarrow CH_3O + e$		3.79(-10)	7.09(-12)	2.81(-13)	1.22(-14)	5.54(-16)	5.09(-17)
$C_2 \rightarrow C + C$		8.03(-11)	2.64(-12)	2.08(-13)	1.96(-14)	2.00(-15)	4.13(-16)
$CH^+ \rightarrow C + H^+$		1.35(-10)	1.61(-12)	4.17(-14)	1.19(-15)	3.57(-17)	2.22(-18)
$NH_2 \rightarrow NH + H$		2.11(-10)	1.87(-11)	2.79(-12)	4.46(-13)	7.51(-14)	2.42(-14)
$CO_2 \rightarrow CO + O$		7.27(-10)	1.48(-11)	7.05(-13)	4.34(-14)	3.49(-15)	6.94(-16)
$O_2 \rightarrow O + O$		3.71(-10)	2.13(-11)	2.31(-12)	2.80(-13)	3.62(-14)	9.36(-15)
$O_2 \rightarrow O_2^+ + e$		3.01(-11)	3.13(-13)	7.07(-15)	1.72(-16)	4.31(-18)	2.18(-19)
$CH \rightarrow C + H$		4.70(-10)	3.89(-11)	6.20(-12)	1.19(-12)	2.70(-13)	1.21(-13)
$HCl \rightarrow H + Cl$		5.90(-10)	2.58(-11)	2.40(-12)	2.71(-13)	3.54(-14)	9.70(-15)
$C_4H_2 \rightarrow C_4H + H$		1.00(-09)	6.56(-11)	8.17(-12)	1.15(-12)	1.75(-13)	5.26(-14)
$C_4H_2 \rightarrow C_4H_2^+ + e$		2.45(-10)	5.79(-12)	3.01(-13)	1.79(-14)	1.14(-15)	1.49(-16)
$C_4H_2 \rightarrow C_2H + C_2H$		1.00(-09)	6.56(-11)	8.17(-12)	1.15(-12)	1.75(-13)	5.26(-14)
$NO \rightarrow N + O$		2.35(-10)	1.38(-11)	1.67(-12)	2.34(-13)	3.60(-14)	1.09(-14)
$H_2O \rightarrow H + OH$		3.19(-10)	1.66(-11)	1.88(-12)	2.56(-13)	3.90(-14)	1.20(-14)
$HCN \rightarrow H + CN$		6.81(-10)	2.07(-11)	1.38(-12)	1.12(-13)	1.05(-14)	2.14(-15)
$C_3 \rightarrow C_2 + C$		2.03(-09)	1.45(-10)	1.82(-11)	2.47(-12)	3.49(-13)	9.61(-14)
$CH_5N \rightarrow HCN + H_2 + 2H$		4.63(-10)	1.78(-11)	1.57(-12)	1.78(-13)	2.40(-14)	6.83(-15)
$CH_5N \rightarrow CH_3N + 2H$		4.74(-11)	4.25(-12)	6.40(-13)	1.03(-13)	1.75(-14)	5.69(-15)
$CH_5N \rightarrow CH_3 + NH_2$		2.16(-10)	7.57(-12)	6.18(-13)	6.59(-14)	8.61(-15)	2.41(-15)
$CH_5N \rightarrow CN + 2H_2 + H$		1.19(-10)	4.58(-12)	3.97(-13)	4.34(-14)	5.63(-15)	1.55(-15)
$CH_5N \rightarrow CH_5N^+ + e$		2.45(-10)	5.79(-12)	3.01(-13)	1.79(-14)	1.14(-15)	1.49(-16)
$CH_5N \rightarrow HCN + H_2$		1.90(-09)	1.07(-10)	1.32(-11)	1.91(-12)	3.03(-13)	9.41(-14)
$CH_3OCH_3 \rightarrow H_2CO + CH_4$		7.93(-10)	4.48(-11)	5.40(-12)	7.57(-13)	1.17(-13)	3.56(-14)
$CH_3OCH_3 \rightarrow CH_3OCH_3^+ + e$		2.45(-10)	5.79(-12)	3.01(-13)	1.79(-14)	1.14(-15)	1.49(-16)
$C_3HN \rightarrow C_3H + CN$		3.99(-09)	1.93(-10)	1.82(-11)	1.93(-12)	2.20(-13)	5.03(-14)
$C_2H_4 \rightarrow C_2H_2 + H_2$		1.60(-09)	9.59(-11)	1.19(-11)	1.72(-12)	2.72(-13)	8.49(-14)
$C_2H_4 \rightarrow C_2H_4^+ + e$		1.38(-10)	2.25(-12)	8.09(-14)	3.30(-15)	1.43(-16)	1.28(-17)
$CH_2O_2 \rightarrow HCO + OH$		2.22(-10)	1.13(-11)	1.07(-12)	1.11(-13)	1.21(-14)	2.61(-15)
$CH_2O_2 \rightarrow CH_2O_2^+ + e$		1.42(-10)	2.46(-12)	9.25(-14)	3.90(-15)	1.73(-16)	1.57(-17)
$C_2H_3O \rightarrow CH_2 + CO$		7.65(-10)	5.48(-11)	7.18(-12)	1.04(-12)	1.63(-13)	5.02(-14)
$C_2H_3O \rightarrow C_2H_3O^+ + e$		3.56(-10)	1.09(-11)	7.45(-13)	5.94(-14)	5.14(-15)	9.16(-16)
$C_2H_3N \rightarrow CH_3 + CN$		1.81(-09)	5.41(-11)	3.79(-12)	3.21(-13)	3.02(-14)	5.89(-15)
$C_2H_3N \rightarrow C_2H_3N^+ + e$		3.31(-10)	3.80(-12)	9.26(-14)	2.43(-15)	6.49(-17)	3.50(-18)
$C_2H_2OH \rightarrow C_2H_2 + OH$		1.55(-09)	6.48(-11)	6.17(-12)	7.12(-13)	9.36(-14)	2.55(-14)
$C_2H_2OH \rightarrow C_2H_2OH^+ + e$		5.41(-10)	1.06(-11)	4.73(-13)	2.49(-14)	1.45(-15)	1.77(-16)
$C_2H_4O \rightarrow CH_3 + CHO$		5.97(-10)	5.03(-11)	7.24(-12)	1.12(-12)	1.83(-13)	5.78(-14)
$C_2H_4O \rightarrow CH_4 + CO$		5.97(-10)	5.03(-11)	7.24(-12)	1.12(-12)	1.83(-13)	5.78(-14)
$C_2H_4O \rightarrow C_2H_4O^+ + e$		2.45(-10)	5.79(-12)	3.01(-13)	1.79(-14)	1.14(-15)	1.49(-16)
$C_3O \rightarrow C_2 + CO$		3.80(-09)	2.96(-10)	4.15(-11)	6.36(-12)	1.03(-12)	3.25(-13)
$CN \rightarrow C + N$		5.87(-10)	6.95(-12)	1.75(-13)	4.77(-15)	1.33(-16)	7.47(-18)
$HCO \rightarrow HCO^+ + e$		3.00(-10)	8.36(-12)	5.23(-13)	3.86(-14)	3.14(-15)	5.33(-16)
$HNCO \rightarrow NH + CO$		9.48(-10)	4.84(-11)	4.86(-12)	5.63(-13)	7.28(-14)	1.95(-14)
$C_3H_4 \rightarrow C_3H_3 + H$		1.77(-09)	9.15(-11)	9.25(-12)	1.07(-12)	1.36(-13)	3.58(-14)
$C_3H_4 \rightarrow C_3H_4^+ + e$		1.16(-09)	2.47(-11)	1.18(-12)	6.54(-14)	3.94(-15)	4.95(-16)
$H_2S \rightarrow H_2 + S$		1.57(-09)	5.68(-11)	4.91(-12)	5.29(-13)	6.52(-14)	1.68(-14)
$H_2S \rightarrow H_2S^+ + e$		3.39(-10)	5.55(-12)	2.00(-13)	8.20(-15)	3.57(-16)	3.20(-17)
$OH \rightarrow O + H$		1.90(-10)	8.94(-12)	1.00(-12)	1.35(-13)	2.03(-14)	6.07(-15)

TABLE 2C
 PHOTODISSOCIATION AND PHOTOIONIZATION RATES (s^{-1}) VERSUS A_v FOR A CLOUD WITH $A_v^{tot} = 100$

reaction	$A_v/$	0.0	3.0	6.0	9.0	12.0	15.0
$NO_2 \rightarrow NO + O$		6.64(-10)	6.45(-13)	2.37(-15)	1.05(-17)	4.97(-20)	2.43(-22)
$SO_2 \rightarrow SO + O$		1.01(-09)	4.70(-13)	1.13(-15)	3.99(-18)	1.62(-20)	6.99(-23)
$CS_2 \rightarrow CS + S$		3.78(-09)	4.15(-12)	1.37(-14)	5.14(-17)	2.06(-19)	8.61(-22)
$OCS \rightarrow CO + S$		2.01(-09)	2.27(-12)	8.29(-15)	3.52(-17)	1.60(-19)	7.49(-22)
$OCS \rightarrow OCS^+ + e$		2.27(-10)	3.15(-15)	2.10(-19)	1.97(-23)	2.01(-27)	2.09(-31)
$NH_3 \rightarrow NH_2 + H$		5.85(-10)	4.12(-13)	1.31(-15)	5.19(-18)	2.22(-20)	9.91(-23)
$NH_3 \rightarrow NH_3^+ + e$		9.44(-11)	2.11(-15)	1.76(-19)	1.81(-23)	2.05(-27)	2.46(-31)
$CH_4 \rightarrow CH_2 + H_2$		5.28(-10)	1.11(-13)	9.75(-17)	1.13(-19)	1.54(-22)	2.47(-25)
$H_2O_2 \rightarrow 2OH$		4.49(-10)	2.54(-13)	6.82(-16)	2.54(-18)	1.09(-20)	5.00(-23)
$C_2H_2 \rightarrow C_2H + H$		3.95(-09)	2.57(-12)	5.55(-15)	1.44(-17)	4.13(-20)	1.27(-22)
$C_2H_2 \rightarrow C_2H_2^+ + e$		2.46(-10)	5.38(-15)	4.64(-19)	4.66(-23)	4.83(-27)	5.03(-31)
$H_2CO \rightarrow H_2 + CO$		7.81(-10)	6.59(-13)	2.08(-15)	8.24(-18)	3.59(-20)	1.65(-22)
$CH_3OH \rightarrow CH_3 + OH$		6.30(-10)	3.00(-13)	7.75(-16)	2.75(-18)	1.09(-20)	4.57(-23)
$CH_3OH \rightarrow CH_3O^+ + H + e$		4.97(-12)	3.64(-17)	7.11(-22)	1.42(-26)	2.85(-31)	5.71(-36)
$CH_3OH \rightarrow CH_4O + e$		3.79(-10)	1.22(-14)	1.19(-18)	1.22(-22)	1.27(-26)	1.33(-30)
$C_2 \rightarrow C + C$		8.03(-11)	1.96(-14)	2.19(-17)	2.70(-20)	3.37(-23)	4.23(-26)
$CH^+ \rightarrow C + H^+$		1.35(-10)	1.19(-15)	3.58(-20)	1.45(-24)	7.45(-29)	4.54(-33)
$NH_2 \rightarrow NH + H$		2.11(-10)	4.46(-13)	2.02(-15)	9.47(-18)	4.49(-20)	2.14(-22)
$CO_2 \rightarrow CO + O$		7.27(-10)	4.34(-14)	4.14(-17)	1.11(-19)	3.84(-22)	1.48(-24)
$O_2 \rightarrow O + O$		3.71(-10)	2.80(-13)	6.33(-16)	1.77(-18)	5.68(-21)	2.00(-23)
$O_2 \rightarrow O_2^+ + e$		3.01(-11)	1.72(-16)	2.79(-21)	4.85(-26)	8.90(-31)	1.74(-35)
$CH \rightarrow C + H$		4.70(-10)	1.18(-12)	1.52(-14)	2.92(-16)	6.13(-18)	1.31(-19)
$HCl \rightarrow H + Cl$		5.98(-10)	2.71(-13)	7.20(-16)	2.86(-18)	1.28(-20)	6.04(-23)
$C_4H_2 \rightarrow C_4H + H$		1.00(-09)	1.15(-12)	4.14(-15)	1.75(-17)	7.81(-20)	3.56(-22)
$C_4H_2 \rightarrow C_4H_2^+ + e$		2.45(-10)	1.79(-14)	5.03(-18)	1.63(-21)	5.52(-25)	1.89(-28)
$C_4H_2 \rightarrow C_2H + C_2H$		1.00(-09)	1.15(-12)	4.14(-15)	1.75(-17)	7.81(-20)	3.56(-22)
$NO \rightarrow N + O$		2.35(-10)	2.34(-13)	8.72(-16)	3.81(-18)	1.76(-20)	8.41(-23)
$H_2O \rightarrow H + OH$		3.19(-10)	2.55(-13)	9.65(-16)	4.42(-18)	2.14(-20)	1.06(-22)
$HCN \rightarrow H + CN$		6.81(-10)	1.12(-13)	1.21(-16)	2.62(-19)	8.42(-22)	3.36(-24)
$C_3 \rightarrow C_2 + C$		2.03(-09)	2.47(-12)	6.78(-15)	1.94(-17)	5.56(-20)	1.60(-22)
$CH_2N \rightarrow HCN + H_2 + 2H$		4.63(-10)	1.77(-13)	5.28(-16)	2.28(-18)	1.08(-20)	5.33(-23)
$CH_3N \rightarrow CH_3N + 2H$		4.74(-11)	1.03(-13)	4.78(-16)	2.31(-18)	1.13(-20)	5.62(-23)
$CH_3N \rightarrow CH_3 + NH_2$		2.16(-10)	6.59(-14)	1.85(-16)	8.00(-19)	3.80(-21)	1.87(-23)
$CH_3N \rightarrow CN + 2H_2 + H$		1.19(-10)	4.34(-14)	1.16(-16)	4.78(-19)	2.23(-21)	1.09(-23)
$CH_3N \rightarrow CH_3N^+ + e$		2.45(-10)	1.79(-14)	5.03(-18)	1.63(-21)	5.52(-25)	1.89(-28)
$CH_3N \rightarrow HCN + H_2$		1.90(-09)	1.91(-12)	7.65(-15)	3.50(-17)	1.68(-19)	8.18(-22)
$CH_3OCH_3 \rightarrow H_2CO + CH_4$		7.93(-10)	7.57(-13)	2.84(-15)	1.24(-17)	5.72(-20)	2.69(-22)
$CH_3OCH_3 \rightarrow CH_3OCH_3^+ + e$		2.45(-10)	1.79(-14)	5.03(-18)	1.63(-21)	5.52(-25)	1.89(-28)
$C_3HN \rightarrow C_2H + CN$		3.99(-09)	1.93(-12)	3.00(-15)	5.83(-18)	1.36(-20)	3.76(-23)
$C_2H_4 \rightarrow C_2H_2 + H_2$		1.60(-09)	1.72(-12)	6.94(-15)	3.23(-17)	1.58(-19)	7.84(-22)
$C_2H_4 \rightarrow C_2H_4^+ + e$		1.38(-10)	3.30(-15)	2.94(-19)	2.98(-23)	3.09(-27)	3.22(-31)
$CH_2O_2 \rightarrow HCO + OH$		2.22(-10)	1.11(-13)	1.45(-16)	2.11(-19)	3.36(-22)	6.05(-25)
$CH_2O_2 \rightarrow CH_2O_2^+ + e$		1.42(-10)	3.90(-15)	3.63(-19)	3.71(-23)	3.86(-27)	4.03(-31)
$C_2H_2O \rightarrow CH_2 + CO$		7.65(-10)	1.04(-12)	4.03(-15)	1.80(-17)	8.44(-20)	4.07(-22)
$C_2H_2O \rightarrow C_2H_2O^+ + e$		3.56(-10)	5.93(-14)	4.23(-17)	3.61(-20)	3.26(-23)	3.00(-26)
$C_2H_3N \rightarrow CH_3 + CN$		1.81(-09)	3.21(-13)	3.03(-16)	4.27(-19)	9.68(-22)	3.35(-24)
$C_2H_3N \rightarrow C_2H_3N^+ + e$		3.31(-10)	2.43(-15)	4.74(-20)	9.47(-25)	1.90(-29)	3.81(-34)
$C_2H_4OH \rightarrow C_2H_4 + OH$		1.55(-09)	7.12(-13)	1.88(-15)	7.41(-18)	3.41(-20)	1.66(-22)
$C_2H_4OH \rightarrow C_2H_4OH^+ + e$		5.41(-10)	2.49(-14)	5.65(-18)	1.70(-21)	5.59(-25)	1.90(-28)
$C_2H_4O \rightarrow CH_3 + CHO$		5.97(-10)	1.12(-12)	4.71(-15)	2.09(-17)	9.48(-20)	4.34(-22)
$C_2H_4O \rightarrow CH_4 + CO$		5.97(-10)	1.12(-12)	4.71(-15)	2.09(-17)	9.48(-20)	4.34(-22)
$C_2H_4O \rightarrow C_2H_4O^+ + e$		2.45(-10)	1.79(-14)	5.03(-18)	1.63(-21)	5.52(-25)	1.89(-28)
$C_3O \rightarrow C_2 + CO$		3.80(-09)	6.35(-12)	2.64(-14)	1.17(-16)	5.32(-19)	2.44(-21)
$CN \rightarrow C + N$		5.87(-10)	4.77(-15)	1.06(-19)	2.46(-24)	5.84(-29)	1.41(-33)
$HCO \rightarrow HCO^+ + e$		3.00(-10)	3.86(-14)	2.36(-17)	1.89(-20)	1.66(-23)	1.51(-26)
$HNCO \rightarrow NH + CO$		9.48(-10)	5.63(-13)	1.41(-15)	5.36(-18)	2.40(-20)	1.14(-22)
$C_3H_4 \rightarrow C_3H_3 + H$		1.77(-09)	1.07(-12)	2.53(-15)	9.00(-18)	3.96(-20)	1.91(-22)
$C_3H_4 \rightarrow C_3H_4^+ + e$		1.16(-09)	6.54(-14)	1.62(-17)	5.01(-21)	1.67(-24)	5.68(-28)
$H_2S \rightarrow H_2 + S$		1.57(-09)	5.28(-13)	1.16(-15)	3.81(-18)	1.50(-20)	6.50(-23)
$H_2S \rightarrow H_2S^+ + e$		3.39(-10)	8.20(-15)	7.34(-19)	7.44(-23)	7.72(-27)	8.05(-31)
$OH \rightarrow O + H$		1.90(-10)	1.35(-13)	4.77(-16)	2.01(-18)	9.08(-21)	4.24(-23)

TABLE 3A

PHOTODISSOCIATION AND PHOTOIONIZATION FITS VERSUS A_v
FOR A CLOUD WITH $A_v^{\text{tot}} = 1$: $\Gamma = C \exp(-\alpha A_v - \beta A_v^2)$

reaction	C (s ⁻¹)	α	β
NO ₂ → NO + O	6.889(-10)	4.218	-4.511
SO ₂ → SO + O	1.032(-09)	4.727	-4.983
CS ₂ → CS + S	3.937(-09)	3.995	-4.286
OCS → CO + S	2.091(-09)	4.045	-4.343
OCS → OCS ⁺ + e	2.261(-10)	6.863	-6.778
NH ₃ → NH ₂ + H	6.013(-10)	4.538	-4.819
NH ₃ → NH ₃ ⁺ + e	9.420(-11)	6.532	-6.518
CH ₄ → CH ₃ + H	5.357(-10)	5.198	-5.407
H ₂ O ₂ → 2OH	4.607(-10)	4.634	-4.902
C ₂ H ₂ → C ₂ H + H	4.080(-09)	4.369	-4.644
C ₂ H ₂ → C ₂ H ₂ ⁺ + e	2.454(-10)	6.591	-6.568
H ₂ CO → H ₂ + CO	8.086(-10)	4.261	-4.547
CH ₃ OH → CH ₃ + OH	6.442(-10)	4.824	-5.083
CH ₃ OH → CH ₃ O ⁺ + H + e	4.943(-12)	7.093	-6.941
CH ₃ OH → CH ₄ O + e	3.789(-10)	6.254	-6.288
C ₂ → C + C	8.120(-11)	5.389	-5.615
CH ⁺ → C + H ⁺	1.344(-10)	7.046	-6.914
NH ₂ → NH + H	2.253(-10)	3.319	-3.600
CO ₂ → CO + O	7.278(-10)	6.155	-6.227
O ₂ → O + O	3.848(-10)	4.198	-4.476
O ₂ → O ₂ ⁺ + e	2.991(-11)	7.271	-7.082
CH → C + H	4.979(-10)	3.550	-3.850
HCl → H + Cl	6.112(-10)	4.801	-5.055
C ₄ H ₂ → C ₄ H + H	1.046(-09)	3.964	-4.254
C ₄ H ₂ → C ₄ H ₂ ⁺ + e	2.461(-10)	5.887	-6.005
C ₄ H ₂ → C ₂ H + C ₂ H	1.046(-09)	3.964	-4.254
NO → N + O	2.431(-10)	4.240	-4.537
H ₂ O → H + OH	3.283(-10)	4.481	-4.766
HCN → H + CN	6.880(-10)	5.427	-5.607
C ₃ → C ₂ + C	2.135(-09)	3.741	-4.023
CH ₂ N → HCN + H ₂ + 2H	4.706(-10)	5.036	-5.272
CH ₂ N → CH ₃ N + 2H	5.059(-11)	3.289	-3.569
CH ₃ N → CH ₃ + NH ₂	2.188(-10)	5.197	-5.412
CH ₃ N → CN + 2H ₂ + H	1.212(-10)	5.029	-5.265
CH ₃ N → CH ₃ N ⁺ + e	2.461(-10)	5.887	-6.005
CH ₃ N → HCN + H ₂	1.968(-09)	4.402	-4.716
CH ₃ OCH ₃ → H ₂ CO + CH ₄	8.205(-10)	4.342	-4.644
CH ₃ OCH ₃ → CH ₃ OCH ₃ ⁺ + e	2.461(-10)	5.887	-6.005
C ₃ HN → C ₂ H + CN	4.104(-09)	4.542	-4.808
C ₂ H ₄ → C ₂ H ₂ + H ₂	1.660(-09)	4.207	-4.510
C ₂ H ₄ → C ₂ H ₄ ⁺ + e	1.379(-10)	6.526	-6.518
CH ₂ O ₂ → HCO + OH	2.291(-10)	4.410	-4.676
CH ₂ O ₂ → CH ₂ O ₂ ⁺ + e	1.414(-10)	6.406	-6.419
C ₂ H ₂ O → CH ₂ + CO	8.037(-10)	3.771	-4.060
C ₂ H ₂ O → C ₂ H ₂ O ⁺ + e	3.595(-10)	5.439	-5.632
C ₂ H ₃ N → CH ₃ + CN	1.823(-09)	5.523	-5.717
C ₂ H ₃ N → C ₂ H ₃ N ⁺ + e	3.295(-10)	7.094	-6.942
C ₂ H ₃ OH → C ₂ H ₃ + OH	1.582(-09)	4.922	-5.188
C ₂ H ₃ OH → C ₂ H ₃ OH ⁺ + e	5.412(-10)	6.227	-6.287
C ₂ H ₄ O → CH ₃ + CHO	6.339(-10)	3.417	-3.700
C ₂ H ₄ O → CH ₄ + CO	6.339(-10)	3.417	-3.700
C ₂ H ₄ O → C ₂ H ₄ O ⁺ + e	2.461(-10)	5.887	-6.005
C ₃ O → C ₂ + CO	4.008(-09)	3.612	-3.904
CN → C + N	5.833(-10)	7.037	-6.898
HCO → HCO ⁺ + e	3.027(-10)	5.618	-5.786
HNCO → NH + CO	9.768(-10)	4.428	-4.697
C ₃ H ₄ → C ₃ H ₃ + H	1.830(-09)	4.416	-4.687
C ₃ H ₄ → C ₃ H ₄ ⁺ + e	1.162(-09)	6.071	-6.158
H ₂ S → H ₂ + S	1.593(-09)	5.204	-5.445
H ₂ S → H ₂ S ⁺ + e	3.377(-10)	6.515	-6.510
OH → O + H	1.949(-10)	4.764	-5.059

TABLE 3B

PHOTODISSOCIATION AND PHOTOIONIZATION FITS VERSUS A_v
FOR A CLOUD WITH $A_v^{\text{tot}} = 10$: $\Gamma = C \exp(-\alpha A_v - \beta A_v^2)$

reaction	C (s ⁻¹)	α	β
NO ₂ → NO + O	5.721(-10)	2.728	-1.461(-01)
SO ₂ → SO + O	8.674(-10)	3.023	-1.628(-01)
CS ₂ → CS + S	3.303(-09)	2.643	-1.302(-01)
OCS → CO + S	1.742(-09)	2.649	-1.358(-01)
OCS → OCS ⁺ + e	1.890(-10)	4.168	-1.559(-01)
NH ₃ → NH ₂ + H	4.956(-10)	2.869	-1.582(-01)
NH ₃ → NH ₃ ⁺ + e	7.862(-11)	3.967	-1.415(-01)
CH ₄ → CH ₃ + H	4.489(-10)	3.250	-1.503(-01)
H ₂ O ₂ → 2OH	3.836(-10)	2.947	-1.592(-01)
C ₂ H ₂ → C ₂ H + H	3.970(-09)	2.925	-1.544(-01)
C ₂ H ₂ → C ₂ H ₂ ⁺ + e	2.036(-10)	3.987	-1.463(-01)
H ₂ CO → H ₂ + CO	6.765(-10)	2.771	-1.443(-01)
CH ₃ OH → CH ₃ + OH	5.329(-10)	3.031	-1.688(-01)
CH ₃ OH → CH ₃ O ⁺ + H + e	4.111(-12)	4.276	-1.213(-01)
CH ₃ OH → CH ₄ O + e	3.166(-10)	3.809	-1.295(-01)
C ₂ → C + C	7.424(-11)	3.336	-1.825(-01)
CH ⁺ → C + H ⁺	1.120(-10)	4.255	-1.347(-01)
NH ₂ → NH + H	2.071(-10)	2.442	-1.241(-01)
CO ₂ → CO + O	7.024(-10)	3.981	-2.409(-01)
O ₂ → O + O	3.256(-10)	2.766	-1.290(-01)
O ₂ → O ₂ ⁺ + e	2.477(-11)	4.367	-1.248(-01)
CH → C + H	4.552(-10)	2.535	-1.761(-01)
HCl → H + Cl	5.698(-10)	3.150	-1.894(-01)
C ₄ H ₂ → C ₄ H + H	8.793(-10)	2.639	-1.333(-01)
C ₄ H ₂ → C ₄ H ₂ ⁺ + e	2.041(-10)	3.585	-1.459(-01)
C ₄ H ₂ → C ₂ H + C ₂ H	8.793(-10)	2.639	-1.333(-01)
NO → N + O	2.006(-10)	2.717	-1.459(-01)
H ₂ O → H + OH	2.696(-10)	2.836	-1.617(-01)
HCN → H + CN	5.814(-10)	3.406	-1.748(-01)
C ₃ → C ₂ + C	1.977(-09)	2.642	-1.289(-01)
CH ₂ N → HCN + H ₂ + 2H	3.909(-10)	3.169	-1.913(-01)
CH ₂ N → CH ₃ N + 2H	4.306(-11)	2.355	-1.077(-01)
CH ₃ N → CH ₃ + NH ₂	1.826(-10)	3.275	-2.011(-01)
CH ₃ N → CN + 2H ₂ + H	1.011(-10)	3.174	-1.865(-01)
CH ₃ N → CH ₃ N ⁺ + e	2.041(-10)	3.585	-1.459(-01)
CH ₃ N → HCN + H ₂	1.592(-09)	2.728	-1.518(-01)
CH ₃ OCH ₃ → H ₂ CO + CH ₄	6.720(-10)	2.743	-1.500(-01)
CH ₃ OCH ₃ → CH ₃ OCH ₃ ⁺ + e	2.041(-10)	3.585	-1.459(-01)
C ₃ HN → C ₂ H + CN	3.829(-09)	3.017	-1.522(-01)
C ₂ H ₄ → C ₂ H ₂ + H ₂	1.367(-09)	2.695	-1.467(-01)
C ₂ H ₄ → C ₂ H ₄ ⁺ + e	1.144(-10)	3.948	-1.431(-01)
CH ₂ O ₂ → HCO + OH	1.945(-10)	2.874	-1.198(-01)
CH ₂ O ₂ → CH ₂ O ₂ ⁺ + e	1.176(-10)	3.883	-1.370(-01)
C ₂ H ₂ O → CH ₂ + CO	6.795(-10)	2.562	-1.261(-01)
C ₂ H ₂ O → C ₂ H ₂ O ⁺ + e	2.969(-10)	3.332	-1.534(-01)
C ₂ H ₃ N → CH ₃ + CN	1.489(-09)	3.352	-1.678(-01)
C ₂ H ₃ N → C ₂ H ₃ N ⁺ + e	2.741(-10)	4.276	-1.213(-01)
C ₂ H ₃ OH → C ₂ H ₃ + OH	1.299(-09)	3.049	-1.716(-01)
C ₂ H ₃ OH → C ₂ H ₃ OH ⁺ + e	4.484(-10)	3.781	-1.602(-01)
C ₂ H ₄ O → CH ₃ + CHO	5.393(-10)	2.412	-1.107(-01)
C ₂ H ₄ O → CH ₄ + CO	5.393(-10)	2.412	-1.107(-01)
C ₂ H ₄ O → C ₂ H ₄ O ⁺ + e	2.041(-10)	3.585	-1.459(-01)
C ₃ O → C ₂ + CO	3.373(-09)	2.470	-1.185(-01)
CN → C + N	5.528(-10)	4.363	-1.463(-01)
HCO → HCO ⁺ + e	2.505(-10)	3.437	-1.593(-01)
HNCO → NH + CO	8.308(-10)	2.902	-1.480(-01)
C ₃ H ₄ → C ₃ H ₃ + H	1.552(-09)	2.885	-1.440(-01)
C ₃ H ₄ → C ₃ H ₄ ⁺ + e	9.646(-10)	3.693	-1.534(-01)
H ₂ S → H ₂ + S	1.296(-09)	3.179	-1.811(-01)
H ₂ S → H ₂ S ⁺ + e	2.804(-10)	3.942	-1.425(-01)
OH → O + H	1.558(-10)	2.886	-1.672(-01)

TABLE 3C

PHOTODISSOCIATION AND PHOTOIONIZATION FITS VERSUS A_v
 FOR A CLOUD WITH $A_v^{\text{tot}} = 100$: $\Gamma = C \exp(-\alpha A_v - \beta A_v^2)$

reaction	C (s^{-1})	α	β
$\text{NO}_2 \rightarrow \text{NO} + \text{O}$	3.710(-10)	2.080	-1.485(-02)
$\text{SO}_2 \rightarrow \text{SO} + \text{O}$	5.171(-10)	2.302	-2.296(-02)
$\text{CS}_2 \rightarrow \text{CS} + \text{S}$	2.311(-09)	2.078	-1.199(-02)
$\text{OCS} \rightarrow \text{CO} + \text{S}$	1.188(-09)	2.054	-1.285(-02)
$\text{OCS} \rightarrow \text{OCS}^+ + e$	1.155(-10)	3.466	-1.995(-02)
$\text{NH}_3 \rightarrow \text{NH}_2 + \text{H}$	3.052(-10)	2.160	-1.715(-02)
$\text{NH}_3 \rightarrow \text{NH}_2^+ + e$	5.270(-11)	3.346	-1.584(-02)
$\text{CH}_4 \rightarrow \text{CH}_3 + \text{H}$	2.936(-10)	2.606	-2.027(-02)
$\text{H}_2\text{O}_2 \rightarrow 2\text{OH}$	2.356(-10)	2.247	-2.118(-02)
$\text{C}_2\text{H}_2 \rightarrow \text{C}_2\text{H} + \text{H}$	2.352(-09)	2.246	-1.471(-02)
$\text{C}_2\text{H}_2 \rightarrow \text{C}_2\text{H}_2^+ + e$	1.315(-10)	3.322	-1.344(-02)
$\text{H}_2\text{CO} \rightarrow \text{H}_2 + \text{CO}$	4.436(-10)	2.140	-1.630(-02)
$\text{CH}_3\text{OH} \rightarrow \text{CH}_3 + \text{OH}$	3.116(-10)	2.273	-2.139(-02)
$\text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{O}^+ + \text{H} + e$	3.020(-12)	3.739	-7.036(-03)
$\text{CH}_3\text{OH} \rightarrow \text{CH}_3\text{O} + e$	2.222(-10)	3.229	-8.982(-03)
$\text{C}_2 \rightarrow \text{C} + \text{C}$	3.982(-11)	2.481	-1.308(-02)
$\text{CH}^+ \rightarrow \text{C} + \text{H}^+$	8.116(-11)	3.712	-2.045(-02)
$\text{NH}_2 \rightarrow \text{NH} + \text{H}$	1.460(-10)	1.903	-6.198(-03)
$\text{CO}_2 \rightarrow \text{CO} + \text{O}$	2.658(-10)	2.871	-4.794(-02)
$\text{O}_2 \rightarrow \text{O} + \text{O}$	2.324(-10)	2.227	-1.540(-02)
$\text{O}_2 \rightarrow \text{O}_2^+ + e$	1.823(-11)	3.829	-9.955(-03)
$\text{CH} \rightarrow \text{C} + \text{H}$	2.434(-10)	1.735	-2.212(-02)
$\text{HCl} \rightarrow \text{H} + \text{Cl}$	2.911(-10)	2.286	-2.393(-02)
$\text{C}_4\text{H}_2 \rightarrow \text{C}_4\text{H} + \text{H}$	6.008(-10)	2.054	-1.256(-02)
$\text{C}_4\text{H}_2 \rightarrow \text{C}_4\text{H}_2^+ + e$	1.326(-10)	2.926	-1.331(-02)
$\text{C}_4\text{H}_2 \rightarrow \text{C}_2\text{H} + \text{C}_2\text{H}$	6.008(-10)	2.054	-1.256(-02)
$\text{NO} \rightarrow \text{N} + \text{O}$	1.308(-10)	2.069	-1.397(-02)
$\text{H}_2\text{O} \rightarrow \text{H} + \text{OH}$	1.624(-10)	2.101	-1.634(-02)
$\text{HCN} \rightarrow \text{H} + \text{CN}$	3.444(-10)	2.689	-3.727(-02)
$\text{C}_3 \rightarrow \text{C}_2 + \text{C}$	1.363(-09)	2.075	-6.449(-03)
$\text{CH}_3\text{N} \rightarrow \text{HCN} + \text{H}_2 + 2\text{H}$	2.013(-10)	2.283	-2.498(-02)
$\text{CH}_3\text{N} \rightarrow \text{CH}_3\text{N} + 2\text{H}$	3.292(-11)	1.896	-6.389(-03)
$\text{CH}_3\text{N} \rightarrow \text{CH}_3 + \text{NH}_2$	8.888(-11)	2.335	-2.757(-02)
$\text{CH}_3\text{N} \rightarrow \text{CN} + 2\text{H}_2 + \text{H}$	5.342(-11)	2.321	-2.635(-02)
$\text{CH}_3\text{N} \rightarrow \text{CH}_3\text{N}^+ + e$	1.326(-10)	2.926	-1.331(-02)
$\text{CH}_3\text{N} \rightarrow \text{HCN} + \text{H}_2$	1.017(-09)	2.047	-1.352(-02)
$\text{CH}_3\text{OCH}_3 \rightarrow \text{H}_2\text{CO} + \text{CH}_4$	4.300(-10)	2.070	-1.397(-02)
$\text{CH}_3\text{OCH}_3 \rightarrow \text{CH}_3\text{OCH}_3^+ + e$	1.326(-10)	2.926	-1.331(-02)
$\text{C}_3\text{HN} \rightarrow \text{C}_2\text{H} + \text{CN}$	2.478(-09)	2.377	-1.765(-02)
$\text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_2 + \text{H}_2$	8.857(-10)	2.038	-1.338(-02)
$\text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_4^+ + e$	7.517(-11)	3.299	-1.235(-02)
$\text{CH}_3\text{O}_2 \rightarrow \text{HCO} + \text{OH}$	1.456(-10)	2.375	-1.158(-02)
$\text{CH}_2\text{O}_2 \rightarrow \text{CH}_2\text{O}_2^+ + e$	7.962(-11)	3.265	-1.071(-02)
$\text{C}_2\text{H}_2\text{O} \rightarrow \text{CH}_2 + \text{CO}$	4.797(-10)	2.015	-1.146(-02)
$\text{C}_2\text{H}_2\text{O} \rightarrow \text{C}_2\text{H}_2\text{O}^+ + e$	1.865(-10)	2.639	-1.527(-02)
$\text{C}_2\text{H}_3\text{N} \rightarrow \text{CH}_3 + \text{CN}$	1.003(-09)	2.704	-3.280(-02)
$\text{C}_2\text{H}_3\text{N} \rightarrow \text{C}_2\text{H}_3\text{N}^+ + e$	2.013(-10)	3.739	-7.038(-03)
$\text{C}_2\text{H}_5\text{OH} \rightarrow \text{C}_2\text{H}_5 + \text{OH}$	7.535(-10)	2.288	-2.424(-02)
$\text{C}_2\text{H}_5\text{OH} \rightarrow \text{C}_2\text{H}_5\text{OH}^+ + e$	2.721(-10)	3.058	-1.917(-02)
$\text{C}_2\text{H}_4\text{O} \rightarrow \text{CH}_3 + \text{CHO}$	4.068(-10)	1.938	-7.144(-03)
$\text{C}_2\text{H}_4\text{O} \rightarrow \text{CH}_4 + \text{CO}$	4.068(-10)	1.938	-7.144(-03)
$\text{C}_2\text{H}_4\text{O} \rightarrow \text{C}_2\text{H}_4\text{O}^+ + e$	1.326(-10)	2.926	-1.331(-02)
$\text{C}_3\text{O} \rightarrow \text{C}_2 + \text{CO}$	2.467(-09)	1.956	-8.096(-03)
$\text{CN} \rightarrow \text{C} + \text{N}$	3.555(-10)	3.706	-8.140(-03)
$\text{HCO} \rightarrow \text{HCO}^+ + e$	1.533(-10)	2.722	-1.873(-02)
$\text{HNCO} \rightarrow \text{NH} + \text{CO}$	5.301(-10)	2.266	-2.254(-02)
$\text{C}_3\text{H}_4 \rightarrow \text{C}_3\text{H}_3 + \text{H}$	1.029(-09)	2.283	-2.292(-02)
$\text{C}_3\text{H}_4 \rightarrow \text{C}_3\text{H}_4^+ + e$	6.046(-10)	3.002	-1.668(-02)
$\text{H}_2\text{S} \rightarrow \text{H}_2 + \text{S}$	7.313(-10)	2.375	-2.610(-02)
$\text{H}_2\text{S} \rightarrow \text{H}_2\text{S}^+ + e$	1.847(-10)	3.296	-1.218(-02)
$\text{OH} \rightarrow \text{O} + \text{H}$	9.352(-11)	2.129	-1.664(-02)

to different assumptions about the cross sections. The rates for plane-parallel clouds with $A_v^{\text{tot}} = 1, 10, \text{ and } 100$ are given in Tables 2A–2C. The cross section data were taken from the references listed by Gredel et al. (1989) with the addition of newer data for C_2H_2 (Wu et al. 1989; Smith et al. 1991) and H_2CO (Rogers 1990). We have not considered the photodestruction of species, e.g., H_2 and CO , for which self-shielding in lines is an important effect (cf. van Dishoeck 1988b). The rates given for clouds with $A_v^{\text{tot}} = 100$ are virtually identical to those inside a cloud which is illuminated on one side only. The rates for a particular value of A_v in a cloud illuminated on two sides are nearly equal to the sums of the rates, at the same A_v , inside two clouds illuminated on one side only. As an example, the photodissociation rate of C_2H_2 at $A_v = 5$ in a cloud with $A_v^{\text{tot}} = 10$ is $8.34 \times 10^{-14} \text{ s}^{-1}$, equal to twice the value $4.17 \times 10^{-14} \text{ s}^{-1}$ at $A_v = 5$ in a cloud with $A_v^{\text{tot}} = 100$.

For calculations of the molecular composition of interstellar clouds, simple analytic representations of the depth dependence of the photodestruction rates are useful. We have fitted the calculated photodestruction rates to bi-exponential expressions of the form (van Dishoeck & Dalgarno 1984; van Dishoeck 1986, 1988b)

$$\Gamma_i = C_i \exp(-\alpha_i A_v - \beta_i A_v^2) \text{ s}^{-1},$$

where C_i , α_i , and β_i are parameters depending on the cloud thickness and photodestruction process. Values of the fitting parameters are given in Tables 3A–3C for the molecules considered by Gredel et al. (1989) for clouds with total visual extinctions of 1, 10, and 100 mag. The parameters in Table 3C are chosen to represent the rates into depths corresponding to $A_v = 15$ mag. To proceed to greater depths the parameters α_i and β_i should be replaced by $\alpha'_i = \alpha_i + 7.5 \times \beta_i$ and $\beta'_i = 0$, respectively. The fits are representative of the rates for depths less than $A_v = 15$ and are good to within a factor of about 2 with the largest errors occurring at the surface and near the center of the cloud.

Values of C_i , α_i , and β_i have been calculated by van Dishoeck & Dalgarno (1984) for OH and for many other systems by van Dishoeck (1987, 1988b). These earlier studies applied the method used by Roberge et al. (1981) and used their grain models. The results obtained here are similar to the results of earlier studies for grain model 2 of Roberge et al.

With increasing optical depth, the photodestruction rates become smaller, and beyond some value of A_v , they are negligible compared to the rates due to photons generated by cosmic rays (Prasad & Tarafdar 1983; Sternberg, Dalgarno, & Lepp 1987; Gredel et al. 1989). Even for radiation fields enhanced up to a factor 10^6 over the average interstellar radiation field, cosmic-ray photons dominate beyond $A_v = 12$. Since grains in the outer layers (with $A_v < 25$) of molecular clouds appear to be similar to diffuse cloud grains (Mathis, Mezger, & Panagia 1983), we expect our results to be a reasonable description of molecular clouds with $R = 3.1$.

The rates caused by cosmic rays are uniform through the clouds, except near the boundaries where some of the cosmic-ray generated photons escape. However, attenuated interstellar radiation dominates the boundary regions, and the “edge effect” of the cosmic-ray photons may be ignored. The four parts of Figure 3 compare the cosmic-ray photodestruction rates of

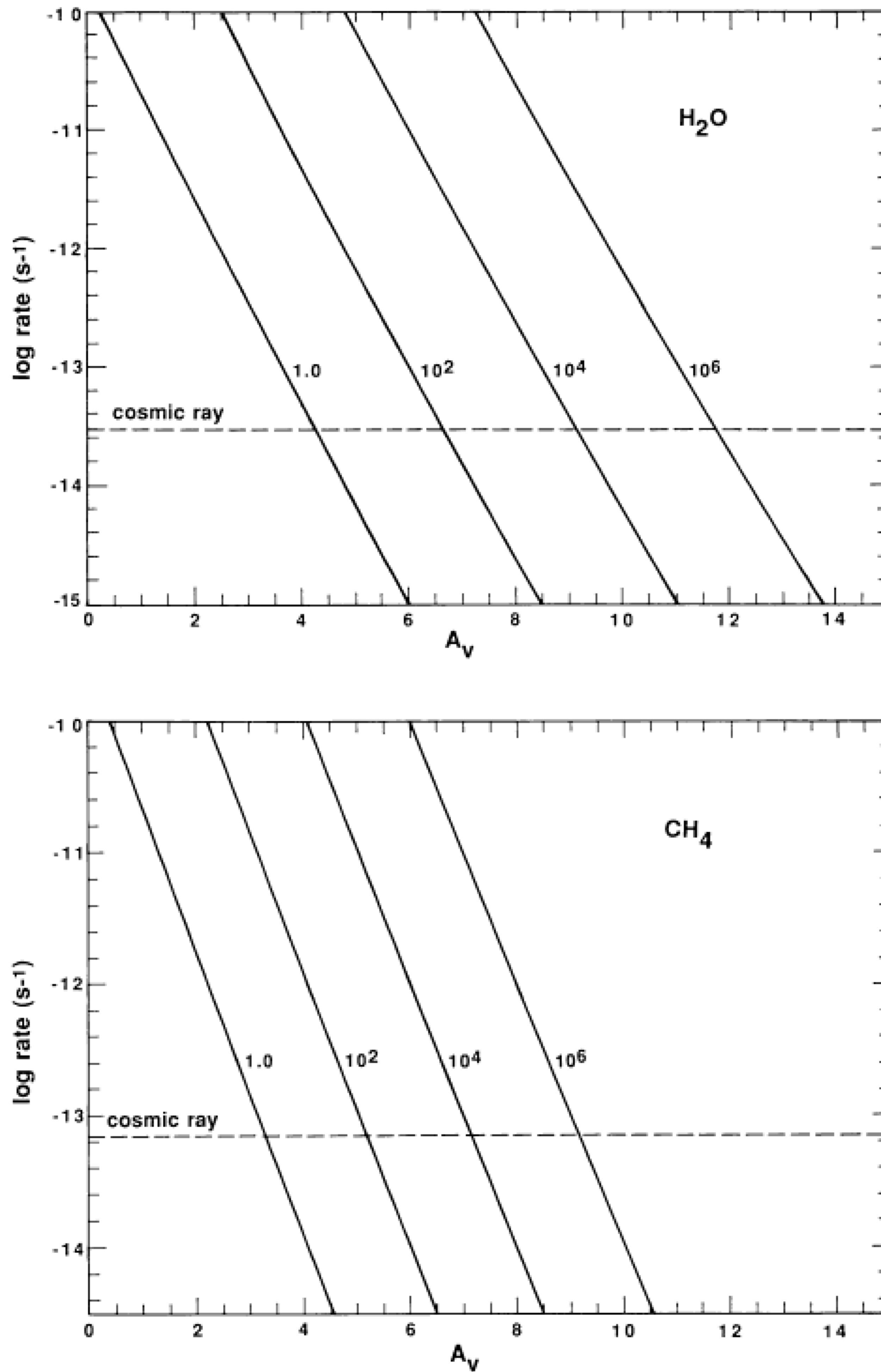


FIG. 3.—The photodestruction rates of H₂O, CH₄, NH₃, and C₂H₂ as functions of A_v for 1.0, 10², 10⁴, and 10⁶ times the standard interstellar radiation field.

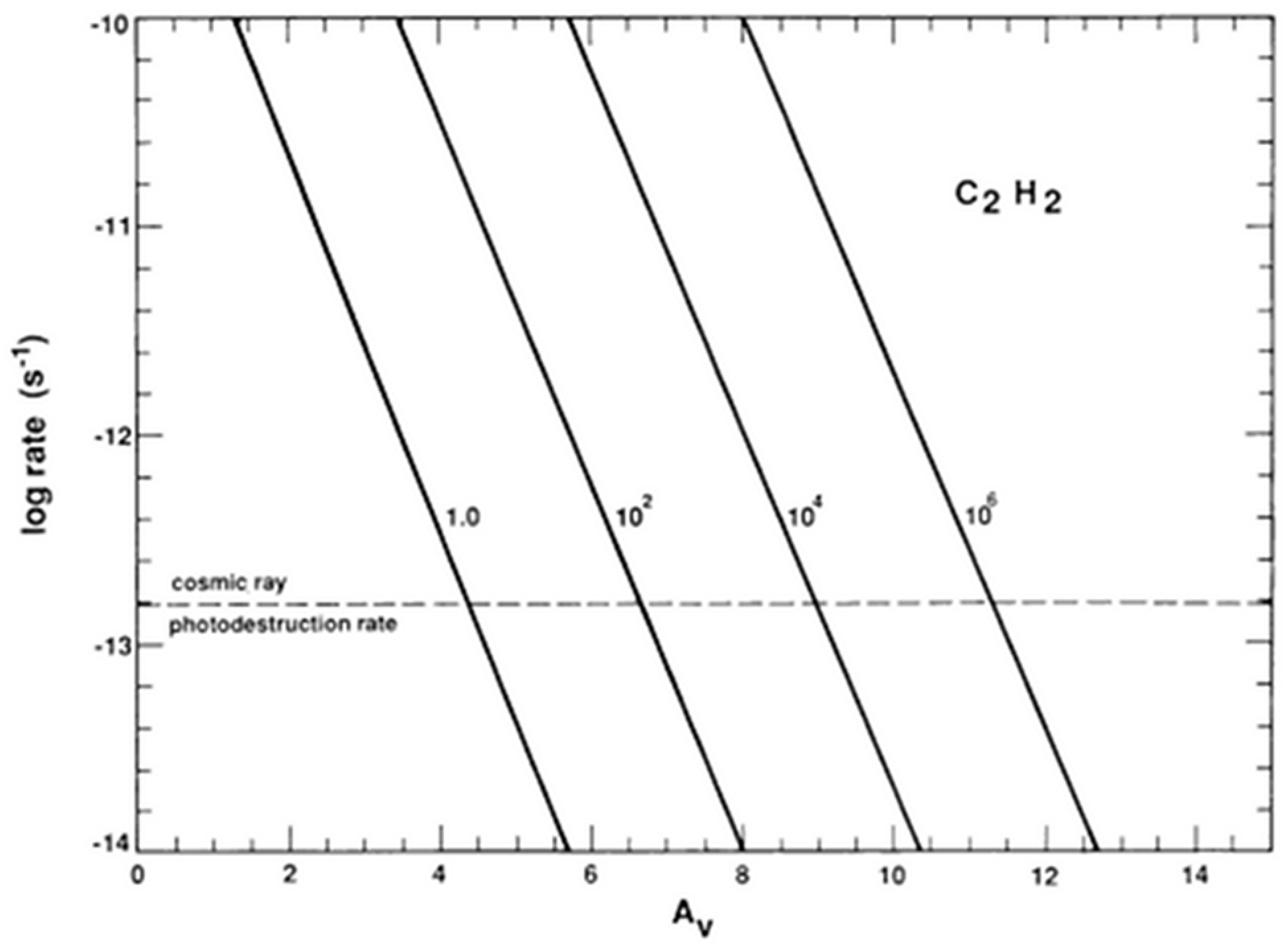
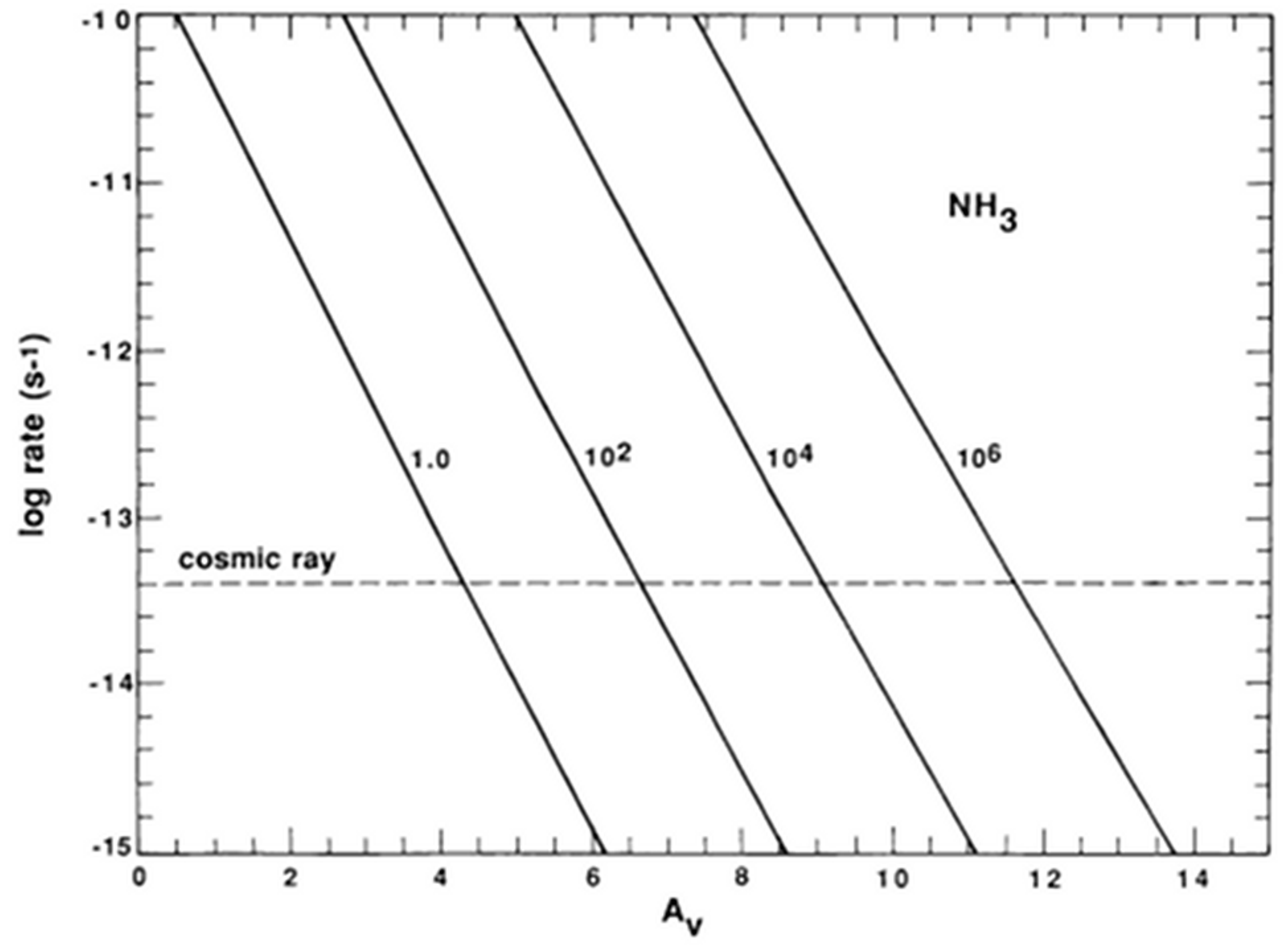


FIG. 3.—Continued

H₂O, CH₄, C₂H₂, and NH₃ (Gredel et al. 1989) with the rates due to the interstellar radiation field, for clouds illuminated by the photons with the same spectrum, but with intensities enhanced by factors between 1 and 10⁶. The figures confirm that even in strong photodissociation regions the cosmic rays dominate photodestruction rates at depths $A_v > 12$.

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REFERENCES

- Aiello, S., Barsella, B., Cecchi-Pestellini, C., Mencaraglia, F., & Rosalie, A. 1987, in IAU Symposium 120, *Astrochemistry*, ed. M. S. Vardya & S. P. Tarafdar (Dordrecht: Reidel), 75
- Bernes, C., & Sandqvist, A. 1977, *ApJ*, 217, 71
- Cardelli, J. A. 1988, *ApJ*, 335, 177
- Cardelli, J. A., Clayton, G. C., & Mathis, J. S. 1989, *ApJ*, 345, 245
- Chlewicki, G., & Greenberg, J. M. 1984, *MNRAS*, 210, 791
- Draine, B. T. 1978, *ApJS*, 36, 595
- Draine, B. T., & Lee, H. M. 1984, *ApJ*, 285, 89
- Flannery, B. P., Roberge, W. G., & Rybicki, G. B. 1980, *ApJ*, 236, 598
- Gredel, R., Lepp, S., Dalgarno, A., & Herbst, E. 1989, *ApJ*, 347, 289
- Herbst, E., & Leung, C. M. 1986, *MNRAS*, 222, 689
- Hollenbach, D. J. 1988, *Ap. Letters Comm.*, 26, 191
- Jackson, J. D. 1975, *Classical Electrodynamics* (2d ed.; New York: Wiley)
- Massa, D., & Savage, B. D. 1989, in IAU Symposium 135, *Interstellar Dust*, ed. L. J. Allamandola & A. G. G. M. Tielens (Dordrecht: Reidel), 3
- Mathis, J. S. 1986, in *The Interrelation of Interstellar, Circumstellar, and Planetary Dust*, ed. J. Nuth & R. Stencel (NASA CP 2403), 29
- Mathis, J. S., Mezger, P. G., & Panagia, N. 1983, *A&A*, 128, 212
- Mathis, J. S., Rimpl, W., & Nordsieck, K. H. 1977, *ApJ*, 217, 425
- Prasad, S. S., & Tarafdar, S. P. 1983, *ApJ*, 267, 603
- Roberge, W. G. 1990, in *Molecular Astrophysics*, ed. T. W. Hartquist (Cambridge: Cambridge Univ. Press), 288
- Roberge, W. G., Dalgarno, A., & Flannery, B. P. 1981, *ApJ*, 243, 817
- Rogers, J. D. 1990, *J. Phys. Chem.*, 94, 4011
- Sandell, G. 1978, *A&A*, 69, 85
- Sandell, G., & Mattila, K. 1975, *A&A*, 42, 357
- Smith, P. L., Yoshino, K., Parkinson, W. H., & Ito, K. 1991, in preparation
- Sternberg, A., Dalgarno, A., & Lepp, S. 1987, *ApJ*, 320, 676
- van Dishoeck, E. F. 1987, in IAU Symposium 120, *Astrochemistry*, ed. M. S. Vardya & S. P. Tarafdar (Dordrecht: Reidel), 51
- . 1988a, in *Millimeter and Submillimeter Astronomy*, ed. W. B. Burton & R. D. Wolstencroft (Dordrecht: Kluwer), 117
- . 1988b, in *Rate Coefficients in Astrochemistry*, ed. T. J. Millar & D. A. Williams (Dordrecht: Kluwer), 49
- van Dishoeck, E. F., & Dalgarno, A. 1984, *ApJ*, 277, 576
- Whitworth, A. P. 1975, *Ap&SS*, 34, 155
- Wu, R. C. Y., Chien, T. S., Liu, G. S., & Judge, D. L. 1989, *J. Chem. Phys.*, 91, 272