CALCULATION OF CHEMICAL EQUILIBRIUM IN THE INTERSTELLAR CLOUD

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ABSTRACT. In order to calculate the molecular concentrations in the interstellar cloud and to obtain their spatial distribution we have made a computational code to solve the set of equations for chemical equilibrium and equations of charge and atom balance. Now 109 molecules and 1070 chemical reactions are included. Besides, the gas phase reactions with neutrals and ions, formation of molecular hydrogen on grains and the ionization and dissociation due to cosmic rays and UV radiation were taken into account. In order to calculate the photodissociation rates of H_2 and CO molecules we take into consideration: i) extinction due to H_2 Lyman and Werner series bands, ii) extinction due to atomic H Lyman series lines — up to n=1 → n=51, iii) extinction due to 33 CO bands and dust continuum extinction. Only UV continuum for photodissociation of all other species was taken into account.

Key words: Interstellar medium: abundances

1. Introduction

One of the most powerful methods to investigate the interstellar medium, particularly the interstellar clouds and inhomogenities near the star forming regions, is the observation of molecular lines. To obtain the physical characteristics of the region, where molecular lines are born, it is necessary to know the distribution of molecular concentrations throughout the cloud. The problem is rather complicated because these concentrations are determined by set of chemical reactions between a great amount of the molecules and atoms. As a result almost all concentrations are mutually dependent. Besides, in many cases the necessity to account for the photochemical reactions leads to modelling of the radiation transfer throughout the cloud. The amount of known interstellar molecules exceeds one hundred. So, the calculations of molecular concentrations in the molecular cloud lead to the set of differential equations if the problem is time–dependent and to the set of algebraical equations for the steady state problem. The latest assumes that the cloud dynamics is unimportant, i.e., that the cloud is stable over the period larger than the chemical timescale. Usually the equilibrium problem is solved, but the unequilibrium approach becomes more and more important in astrophysics. Our experience leads to conclusion that steady state is reached after approximately 10^7 — 10^8 years even for diffuse clouds with total density about 10 cm^{-3}, which is comparable with the clouds' lifetime.

In order to calculate the molecular concentrations in the interstellar cloud with great amount of molecules (more than 100) and chemical reactions (about 1000) it is necessary to have the computer code for solving the set of equations of chemical equilibrium or kinetics with photochemical reactions and radiation transfer, included. There are some such programs in the world, but they are not available in the east European and post Sovietic region (recent exception by Shematovich, Shustov and Wiebe as part of code for calculating the dynamics of protostellar medium). In order to fill up this gap we have made a program package to solve the set of equations of chemical kinetics and equations of charge and atom balance. Now 109 molecules and 1070 chemical reactions are included.

2. The model of the cloud

We assume that the cloud is a plane–parallel slab immersed into Draine's(1978) interstellar ultraviolet radiation field from both sides. It is assumed that no radiaton falls onto cloud shortwards of atomic Lyman limit $\lambda = 911.763$ Å. The cloud is homogenous, isothermic, and the excitation temperatures of all species are equal to the kinetic temperature.

3. Chemical and physical processes taken into account

2.1. Gas phase reactions

The set of chemical reactions by Viala (1986) is used

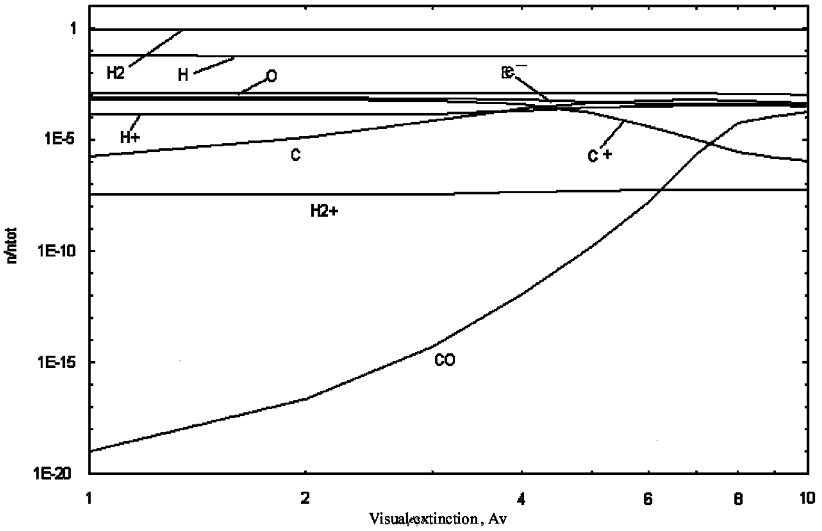

Figure 1: Relative abundances of some species n/n_{total} as function of visual extinction for cloud with total extinction 20, total density 100 cm^{-3} and T$_{kin}$ = 50K.

and 1014 reactions with ions and neutrals are included.

2.2 Formation of the molecular hydrogen on grains

The expression by Viala (1986) is used for the rate R of H_2 formation on grains per H atom:

$$R = 3.6 \cdot 10^{-18} n T^{1/2} \, \mathrm{s}^{-1}$$

where $n = n_H + 2n_{H_2}$ and T is the gas temperature.

2.3 The cosmic rays ionisation rates

They are also taken from Viala's database and all 8 reactions of ionisation H, H_2, He, C, N and O are included.

2.4 The photodissociation, photoionization and radiative transfer

The cloud is assumed to be a plane–parallel slab and exposed in interstellar UV field, approximated by Draine (1978). For all cases except the photodissociation of H_2 and CO only the photodissociation in UV continuum was taken into account, and following Sternberg and Dalgarno (1995) we used the approximation formula:

$$\Gamma_i = 2 \cdot 10^5 C_i \exp(-\alpha_i A_\nu - \beta_i A_\nu^2) s^{-1}$$

where Γ_i is the dissociation rate and C_i, α_i and β_i are the coefficients given in paper by Roberge *et al* (1991). 50 photodissociation reactions are included.

Only the photoionization of atomic carbon and silicon was accounted for. Photoionization rates of Sternberg and Dalgarno (1995) for unattenuated Draine's (1978) UV field were used, multiplying them by attenuation coefficient on dust calculated as in section 2.5.

2.5 Photodissociation of H_2 and CO

In order to calculate the photodissociation rates of H_2 and CO molecules, we assume that the cloud is a plane–parallel slab immersed into Draine's (1978) interstellar ultraviolet radiation field from both sides. It is assumed that no radiation falls onto cloud shortwards of atomic H Lyman limit $\lambda = 911.763$Å. For the purpose of calculation of the mean UV radiation intensity at a given point inside cloud, we account for i) extinction due to H_2 Lyman and Werner series bands, ii) extinction due to atomic H Lyman series lines – up to n=1 → n=51, iii) extinction due to 33 CO bands mentioned by Dishoeck and Black (1988), see Tables I and IV) dust coninuum extinction. The excitation temperatures of all gaseous species are assumed equal to the kinetic temperature, the latter being homogenous throughout the cloud. No scattering in atomic and molecular lines is accounted for; we assume that all the photons absorbed in the ultraviolet are reradiated in the optical and infrared region through cascade processes. Of course, this is not true regarding atomic hydrogen line Ly$_\alpha$, but we use this approximation at the present stage.

Scattering on dust is treated in forward–only scattering approximation, in a manner as by Viala (1986), and we adopted uniform optical properties of dust grains through all the spectral region with UV lines: $911.763\text{Å} \leq \lambda \leq 1250\text{Å}$. As the interstellar extinction curve in far ultraviolet is still quite uncertain, we assume a constant ratio of ultraviolet to visual extinction efficiency, namely, $Q_{UV}^{ext}/Q_V^{ext} = 2.73$ — a little more as in Federman, Glassgold and Kwan (1979), crudely evaluating the curve of Roberge et al. (1991) (see Fig. 1 of this paper). The true dust albedo a_{eff} is assumed to be $a = 0.6$ as by Lillie and Witt (1976), and the effective albedo in forward–only scattering approxima-

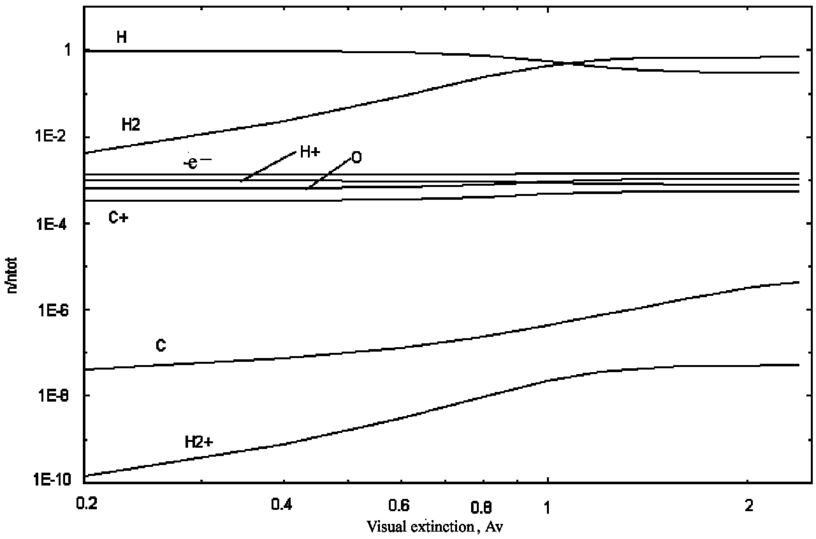

Figure 2: Relative abundances of some species n/n_{total} as function of visual extinction for cloud with total extinction 4.8, total density 20 cm^{-3} and T$_{kin}$ = 50K.

tion:

$$1 - a_{eff} = (1-a)^{1/2}$$

So, the intensity of ultraviolet radiation in pure dust cloud would be described by the formula:

$$I = I_0 \exp(-\tau_V Q_{UV}^{ext}(1-a_{eff})/\mu Q_V^{ext}))$$

where I_0 is the intensity of interstellar UV radiation, τ_V optical depth in the visual region, μ cosine of the angle between the direction of radiation propagation and perpendicular to the slab boundary.

We assume that the mechanism of photodissociation of H_2 is through absorption of UV photons in Lyman and Werner bands, with subsequent dissociation. For H_2 molecular bands each rotational transition line is treated separately, 750 lines in total, assuming Foight profiles for them. Their oscillator strengths and radiative lifetimes were taken from Abgrall and Roueff (1989). For the ground level, 16 lowest rotational sublevels are accounted for, assuming their population to be in accordance with Boltzmann distribution. No collisional processes and turbulence were accounted for i.e. only the thermal motion of gas particles was accounted for to obtain the Doppler widths of line cores for hydrogen and CO.

We calculated the spectral parameters for atomic H lines by exact non–relastivic quantum mechanical treatment (the radial integrals were calculated using method by Hoang–Binh (1990), and Foight profiles were assumed for them, too.

CO molecular bands are treated using more crude approximation, because we have not at our disposal the transition probabilities for individual rotational lines. We use the spectral data of Dishoeck and Black (1988) where the oscillator strengths and radiative lifetimes for vibrational bands as a whole are given, and approximate each of them by Foigt profile of corresponding width.

4. The first results

On to day only a limited set of calculation results with limited number of molecules (36) including only H, O and C is available. Two examples are displayed to show the region of formation of CO (Fig 1) and the region of transition of atomic hydrogen to molecular (Fig 2).

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