A MODEL OF THE CHEMISTRY IN THE NEUTRAL SHELL OF A PLANETARY NEBULA

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A model of the neutral region of a planetary nebula has been constructed, building on an existing program (Abgrall et al. 1992, Astr. Astrophys. 253, 525). It incorporates a large set of equations governing the formation and destruction of molecular species and also covers photo-dissociation/ionization reactions and cosmic ray interactions. The radiation field impinging on the nebula is modelled as a 10^5 K diluted Planck spectrum, truncated below 91.2 nm, augmented by spectral emission lines from the ionized region (data from G. Stasinska, private communication) and the hydrogen (2s→1s) two-photon continuum. The chemical species involved in the reactions are composed of seven elements - H, He, C, O, N, S and Fe - with H and He dominating the elemental abundances. The model considers a chemical environment which is carbon-rich (i.e. $C/O > 1$).

The transfer of radiation in the ultraviolet absorption lines of H_2 and CO is solved in order to accurately determine photodissociation rates for these two important molecular species. For other species the photorates decrease exponentially with optical depth owing to dust absorption and are further reduced through geometrical dilution of the radiation field. Where possible, photorates are calculated more accurately by direct numerical integration of the product of the local photon field strength and the cross-section of the process. This method obviously requires knowledge of the cross-section as a function of wavelength in the relevant wavelength range.

Dust grains cause an exponential decrease in the field intensity which is wavelength dependent. The grains are assumed to be a mixture of silicate and graphite and the wavelength dependence of their absorption coefficient was taken from the literature (Mathis et al. 1983, Astr. Astrophys. 128, 212).

The results of the model show the expected trends in the abundances of major molecular species. Molecular hydrogen and CO rapidly form as the dust optical depth τ_V increases, owing to the efficacity of self-shielding. Recent observations have detected other molecules within planetary nebulae e.g. HCN, HNC and HCO^+ in NGC 2346 (Bachiller et al. 1989, Astr. Astrophys. 210, 366); CN, HCN, HNC and HCO^+ in NGC 7027 (Cox et al. 1992, Astr. Astrophys. in press). The chemical modelling includes these species and many other molecules that may exist in the PN environment, e.g. NH_3, CS, OH, C_2H, C_3H_2, HeH^+. In its present form, the model predicts a column density of HCO^+ of about 10^{12} cm^{-2} at $\tau_V = 5$ compared with a corresponding value of about 10^{21} cm^{-2} for H. For HCN and HNC column densities comparable to HCO^+ are obtained, and for CN a larger value of about 10^{15} cm^{-2} is computed.

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