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THE CHEMISTRY OF PROTOPLANETARY NEBULAE

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ABSTRACT

We discuss three recent attempts at modelling the chemical evolution of the post-AGB phase of stellar evolution, concentrating mostly on the short-lived protoplanetary nebula (PPNe) phase. Although the three models discussed differ in their physical description of PPN, all agree that the high densities, temperatures and UV fluxes can drive a complex organic chemistry on a very short timescale. For instance, O atoms liberated from CO, either by photodissociation or by shock waves, can be converted into OH and H_2O, thereby producing oxygen-bearing molecules in a carbon-rich environment. However, once the molecular region becomes transparent to UV radiation, caused by geometrical dilution if this region is expanding, molecules are quickly destroyed; only the most photo-resistant species, and those which may exist in dense clumps, can survive to the planetary nebula phase.

Key words: Protoplanetary nebulae; astrochemistry.

1. INTRODUCTION

Protoplanetary nebulae are found during a brief stage in the life of a star as it evolves from the Asymptotic Giant Branch (AGB) to become a white dwarf surrounded by a planetary nebula (PN). PPNe can be identified by a high-velocity bipolar shape, with a small, if detectable, ionised region, and the remnants of the lower velocity AGB wind. Their central stars, which may be surrounded by a dense torus, are generally of type B to F, and are evolving rapidly. These stars provide an intense UV radiation field, perhaps 10^4–10^7 times the interstellar field, which interacts with the molecule-rich AGB wind. PPNe are rare objects; this, together with the dynamic ages inferred, lead to the suggestion that they are less than 1 000 yr old, with some perhaps as young as 200 yr.

Molecule-rich PPNe include CRL 2688 and CRL 618. The latter has been well studied by the Infrared Space Observatory (ISO) and a number of complex organic molecules, including the only detection of benzene (C_6H_6) in an object outside the Solar System (Cernicharo et al., 2001a,b), have been observed. Some 20 molecules have been detected in CRL 618, which is a carbon-rich object with the presence of PAH emission and weak silicate bands. Surprisingly, given the presence of molecules such as C_2H_2, C_4H_2, CH_3CCH and CH_3C_4H, the oxygen-bearing molecules OH, H_2O and H_2CO have also been detected (Herpin & Cernicharo, 2000). It has been proposed that these latter molecules are formed from O atoms released either from the photodissociation or the shock-driven destruction of CO. In general terms the molecular composition of PPNe is less complex than that of C-rich AGB stars but more than that of PNe. In addition, molecular abundance ratios which are sensitive to UV flux, in particular the CN/HCN abundance ratio, increase as the central star evolves. A similar result is also found for the HCO^+/HCN ratio, again indicating an increase in the flux of ionising particles as evolution progresses.

In this paper, we review some recently proposed models of PPNe chemistry by concentrating on CRL 618. Nevertheless, we note that PPNe have a wide variety of chemical properties and we present some SEST observations of two southern PPNe which turn out to be molecule poor.

2. MODELLING CRL 618

The ISO observations of CRL 618 made by Cernicharo and collaborators have driven a couple of major investigations of the chemistry which must produce OH and water at the same time as having large abundances of carbon-bearing chain molecules. Two models were developed: the most recent, by Cernicharo (2004), considered a three zone model to capture the essential photo-driven chemistry. This model considered the effects of radiation on a plane-parallel, stationary slabs of gas. Woods et al. (2002, 2003) considered a similar model but allowed the molecular gas to move, thus diluting both the internal number density and ultra-violet extinction as well as the incident UV flux from the central object.

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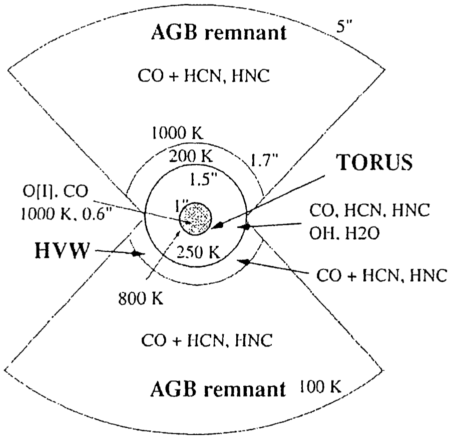

Figure 1. Schematic picture of the chemical structure of CRL 618 (Herpin & Cernicharo, 2000).

CRL 618 consists of a central B0 star with an effective temperature of about 30 000 K surrounded by a compact HII region and a dense torus. Its bipolar outflow has a velocity of $\sim$ 200 km s^{-1} with a remnant AGB envelope expanding at about 20 km s^{-1}. Fig. 1 shows a cartoon of the structure taken from Herpin & Cernicharo (2000). Cernicharo (2004) modelled CRL 618 by considering chemistry within three slabs identical in each of density (10^7 cm^{-3}), temperature (250 K) and thickness (10^{14} cm), but with an extinction taken to be 1, 2 and 3 mags in the three different zones. The lowest extinction slab is assumed to be irradiated by a UV flux some 10^4 times greater than the interstellar flux. The three zones are thus able to crudely simulate a PDR model, with Zone I being the region in which H_2 can be photodissociated; in Zone II H_2, but not CO, self-shields; and in Zone III, both H_2 and CO are shielded. The initial chemical composition of parents in the slabs are taken from observations and models of the AGB phase.

The photodissociation of parent acetylene leads to an extensive organic chemistry with much similarity to that in the circumstellar envelope of IRC+10216. However, the high densities and high UV flux lead to short collisional timescales, on the order of a few seconds, and a very short time to reach a chemical steady-state, on the order of a few years. These models produce peak fractional abundances, $\sim 10^{-6}$, of organic molecules within 1 year and slightly lower steady-state abundances. In Zone II, the photodissociation of CO leads to free oxygen atoms which at high temperatures and at high ionisation are converted into OH, H_2O and H_2CO very efficiently. Thus, by this means one can have a 'mixed' chemistry in a carbon-rich object.

Woods et al. (2002, 2003) proposed a different model for CRL 618, in particular to reproduce the abundance of benzene observed. They modelled the torus by assuming that it could be simulated by a dense, thin shell of gas irradiated by a strong central UV source. They assumed that the shell had constant thickness and allowed it to expand away from the central object at 5 km s^{-1}, thereby undergoing a density decrease as r^{-2} due to geometric dilution. The initial density of the shell was taken as $n(H_2) = 1.6\ 10^9$ cm^{-3} giving an initial extinction intrinsic to the shell of 160 mags, which decreased in proportion to r^{-2} as the shell expanded. The initial abundances were again taken to be those of the parent species in a C-rich AGB star and a temperature of 250 K was adopted. Fig. 2 shows the calculated radial distributions of the fractional abundances of some molecules. In common with the calculations by Cernicharo (2004), the results show that photodissociation of parent molecules drives a very fast and extensive chemistry which effectively builds large hydrocarbon molecules, including benzene. It should be noted here that the Cernicharo (2004) model does not attempt to reproduce the observed abundance of benzene, and that the models of Woods et al. (2002, 2003) do not attempt to reproduce the observed abundances of OH, H_2O and H_2CO.

Chemistry is fast because the collision time at high density is about 1 s, while the rapid drop in abundances seen at around 10^{16} cm is the onset of a 'radiation catastrophe' which occurs once the extinction has fallen to about 10–20 mags. At this point the grains can no longer protect the molecules and they are destroyed rapidly. This result is not so sensitive to the magnitude of the UV flux enhancement, since any linear enhancement is more than offset by the exponential effect of dust shielding. However, the results are sensitive to the expansion velocity chosen for the shell. If the velocity is larger than 5 km s^{-1}, then geometric dilution drives down the extinction so quickly that parent molecules and daughter products are destroyed before they can synthesise larger species. In this sense, the presence of a long-lived, high density torus seems to be essential for the production of abundant complex organic molecules. Fig. 3 compares the observed and calculated column densities. Although many species are in reasonable agreement with observations, including benzene, there are some severe discrepancies, including ethane, which reflects the difficulty in hydrogenating carbon-bearing molecules, and HCO^+ - despite adopting a cosmic ray ionisation flux enhanced by a factor of 500 over the standard interstellar value. This failure to reproduce the HCO^+ abundance is also a feature of chemical models of planetary nebulae.

Nevertheless, based on these two distinct models for CRL 618 we can make some broad conclusions. First, the high densities allow for short collision times between reactive species, both ions and neutrals. Second, the high UV flux must be reduced by grain extinction to a level at which it generates radicals from parents and promotes chemistry. Third, in order for grains to provide extinction sufficient for molecular complexity to develop, the molecular region must be stationary or at least expanding at a velocity much

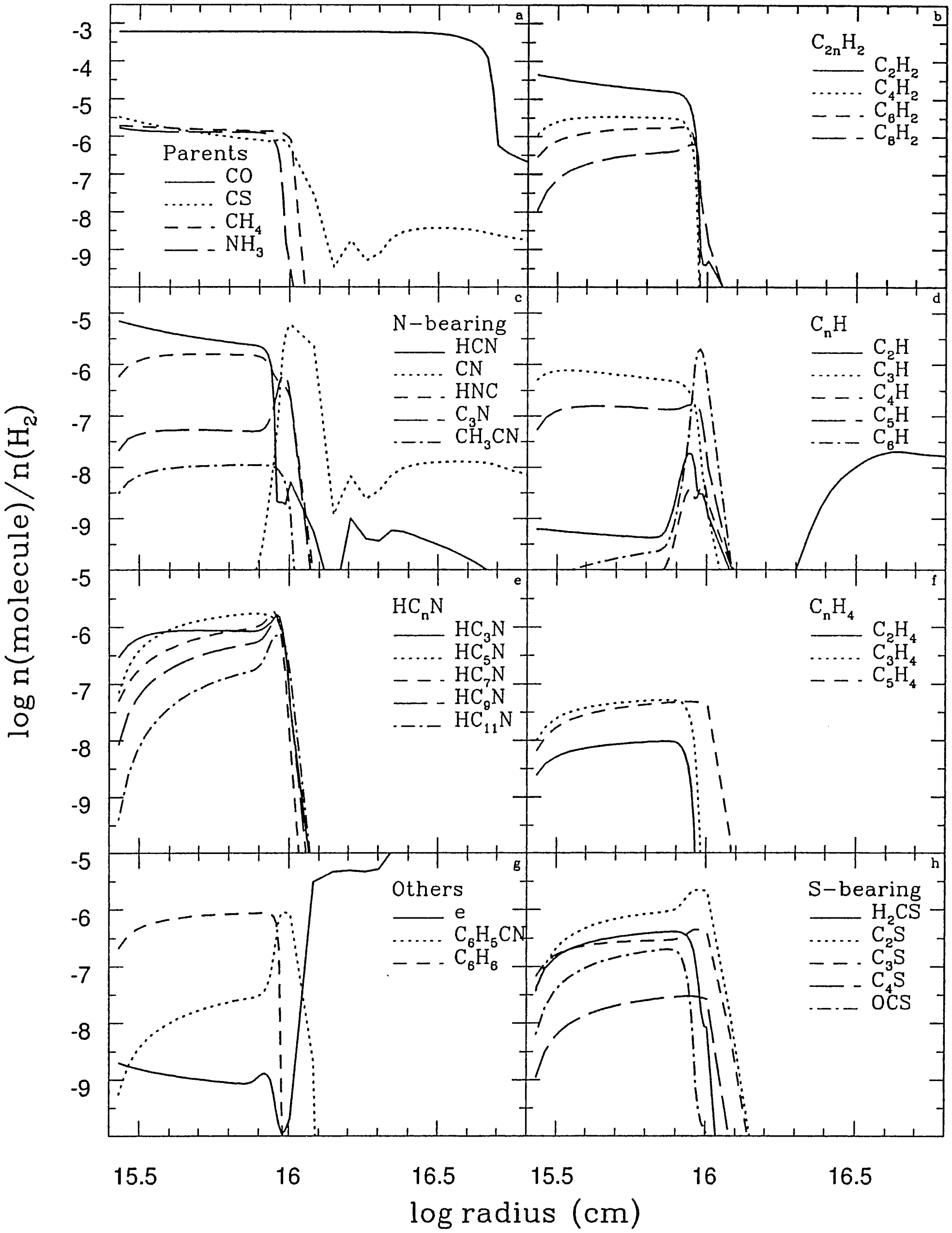

Figure 2. Radial abundances relative to H_2 calculated by Woods et al. (2003) for the molecule-rich CRL 618 model.

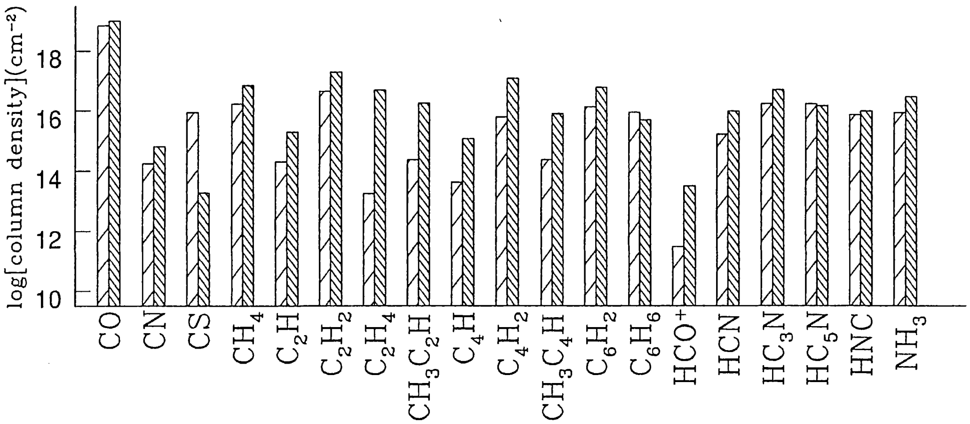

Figure 3. Observed (heavy hashing) and model (light hashing) column densities for molecules in CRL 618 (Woods et al., 2003).

below that of the remnant circumstellar envelope. If these conditions are met, then PPNe can be a site of significant production for complex organic molecules.

3. OTHER PPNE

Since lifetimes are short, PPNe are rare objects and molecule-rich PPNe even rarer. In an attempt to detect counterparts of CRL 618, Woods et al. (2004) undertook with the SEST a selected spectral line survey of two southern bipolar PPNe, IRAS 16594-4656 and IRAS 17150-3224, which are thought to be younger than 400 yr. These PPNe show no evidence of a torus and turn out to have a very poor molecular composition. In addition to CO, only CN and HCN were detected. Woods et al. (2004) have developed a third model for these sources. Since they do not have a dense torus, Woods et al. considered the effect of the central star on the expanding AGB envelope once the mass-loss in the AGB phase had stopped. Thus they modelled the effects of a strong UV flux on the entire AGB CSE as it drifted away at $14\,\mathrm{km\,s^{-1}}$, a typical value for AGB wind velocities, with a mass-loss rate of $10^{-5}\,\mathrm{M_{\odot}\,yr^{-1}}$. The initial conditions for the abundances were found by calculating the molecular distributions expected in a carbon-rich CSE (Fig. 4).

As well as an enhanced internal UV field, they also adopted an enhanced cosmic-ray ionisation rate and X-ray ionisation, allowing the temperature at the interior of the AGB envelope to increase with time, as the central star heats up, while decreasing with radius due to adiabatic cooling. Fig. 5 shows snapshots of particular molecular abundances as a function of radial distance from the central star when the inner edge of the expanding AGB envelope is at (1, 3, 10, 30, 100) 10^{15} cm, that is, views of the envelope over a period of about 2 000 yr. The plotted fractional abundances show that for timescales longer than about 800 yr, only CO is abundant in the envelope. The lower row of Fig. 5 shows the variation in CN/HCN, HNC/HCN and HCN/CO abundance ratios.

4. CONCLUSIONS

Molecular line observations of PPNe have been revolutionised by the use of the ISO Long-Wavelength Spectrometer by Cernicharo and co-workers. Their observations extended the range of molecules detected to hydrocarbon species, including non-polar species. However, detailed studies are essentially limited to one PPN, CRL 618. Although the spatial resolution of ISO was limited, detailed excitation analysis has enabled a number of different molecule-rich regions to be detected. As a result, there have been a small number of chemical models developed to explain the observations. One should note that these models should be treated with some caution - there is as yet no consensus on the detailed physics to be included, for example the models by Cernicharo (2004) and Woods et al. (2002) include stellar UV fields which differ by a factor of 320. Furthermore, Cernicharo adopts a stationary cloud model with constant physical conditions and a maximum visual extinction of 3 mags; Woods et al. (2002) consider a constant thickness torus which drifts away from the central star, so that the density and extinction vary as r^{-2}. This model thus starts with a very high visual extinction. Even so, the high UV flux allows some parent species, particularly C_2H_2, to be photodissociated and the short collision timescales then build up large abundances of hydrocarbons very rapidly. For example, the model predicts a large abundance of benzene in agreement with the observations. Complex molecules remain abundant until the visual extinction falls to less than about 20 mags, at which point the fast photo-rates destroy all molecules rapidly. Woods et al. (2002) found out

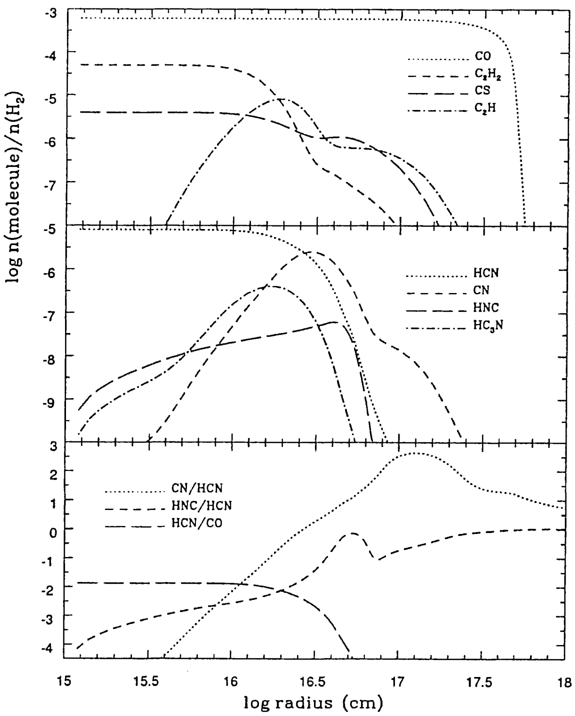

Figure 4. Radial abundances relative to H_2 calculated by Woods et al. (2003) for a carbon-rich CSE.

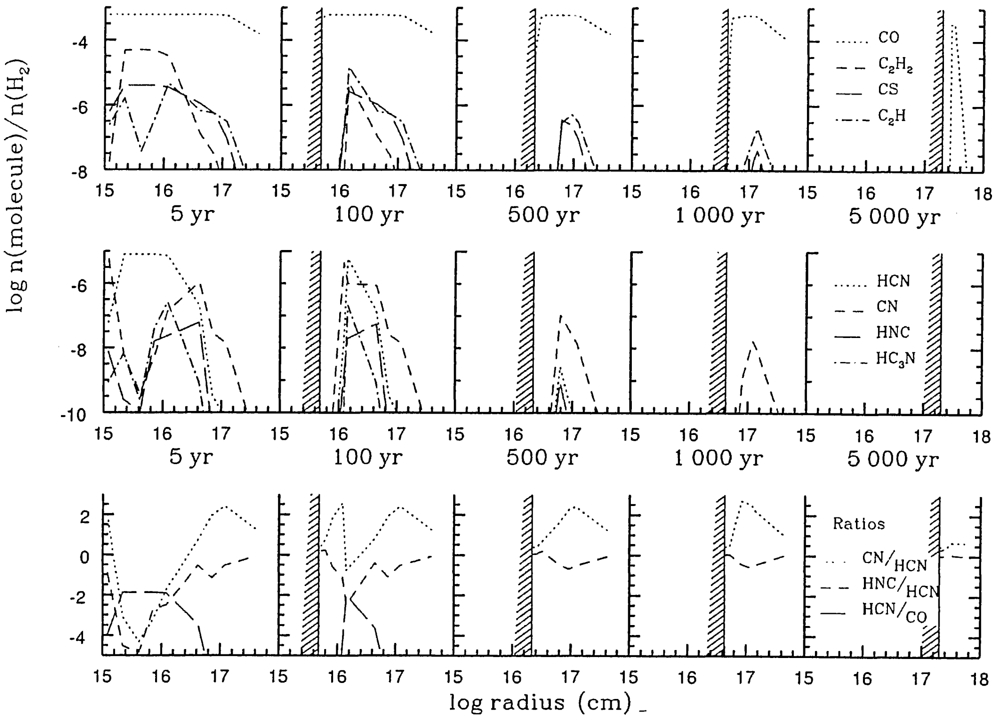

Figure 5. IRAS 16594-4656: Radial abundance profiles for particular molecules at various instances as the AGB envelope drifts away from the central star. The hatched area marks out the position of the inner edge of the AGB circumstellar envelope (Woods et al., 2004).

that the drift velocity of the torus had to be small otherwise its number density and UV extinction fall so rapidly that complex molecules cannot be formed in abundance. The presence of a torus, or a quasi-stationary layer, thus appears to be essential for complex molecule formation.

Indeed, the models by Woods et al. (2004), which do not include a torus and instead consider the interaction of the central UV field with an expanding AGB circumstellar shell, show that parent molecules are destroyed rapidly and very little complexity ensues.

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