Mon. Not. R. Astron. Soc. **325,** 881–885 (2001)

Gas-phase models for the evolved planetary nebulae NGC 6781, M4-9 and NGC 7293

A. Ali,[1] O. M. Shalabiea,[1,2] M. S. El-Nawawy[1] and T. J. Millar[3]★

[1]*Cairo University, Faculty of Science, Astronomy Department, Giza, Egypt*
[2]*Astronomy Program, SEES, Seoul National University, Seoul 151-742, Korea*
[3]*Department of Physics, UMIST, PO Box 88, Manchester M60 1QD*

Accepted 2001 March 15. Received 2001 March 15; in original form 2000 October 30

ABSTRACT

We have studied the chemistry of the molecular gas in evolved planetary nebulae. Three pseudo-time-dependent gas-phase models have been constructed for dense (10^4–10^5 cm^{-3}) and cool ($T \sim 15$ K) clumpy envelopes of the evolved nebulae NGC 6781, M4-9 and NGC 7293. The three nebulae are modelled as carbon-rich stars evolved from the asymptotic giant branch to the late planetary nebula phase. The clumpy neutral envelopes are subjected to ultraviolet radiation from the central star and X-rays that enhance the rate of ionization in the clumps. With the ionization rate enhanced by four orders of magnitude over that of the ISM, we find that resultant abundances of the species HCN, HNC, HC_3N and SiC_2 are in good agreement with observations, while those of CN, HCO^+, CS and SiO are in rough agreement. The results indicate that molecular species such as CH, CH_2, CH_2^+, HCl, OH and H_2O are anticipated to be highly abundant in these objects.

Key words: ISM: molecules – planetary nebulae: general – planetary nebulae: individual: NGC 6781 – planetary nebulae: individual: M4-9 – planetary nebulae: individual: NGC 7293 (Helix Nebula).

1 INTRODUCTION

The presence of neutral matter in planetary nebulae (PNe) is now well established. The observations confirm that the chemical composition of the molecular gas in PNe is radically different from that in interstellar clouds and the circumstellar envelopes of asymptotic giant branch (AGB) stars. The molecular envelopes of PNe form from highly fragmented, spheroidal shells or rings around the ionized nebulae.

The CO and H_2 observations of the Helix nebula (NGC 7293) imply the existence of a substantial quantity of cool, molecular gas, perhaps in the form of dense, shielded clumps (Bachiller et al. 1989a,b, 1993; Kastner et al. 1996). These clumps have a cometary shape with a tail pointing away from the central star. Meaburn et al. (1992) estimated the mean gas density (n_H) in the clumps to be $\sim 6.2 \times 10^5$ cm^{-3}, from the equation $N(H + H_2)/E(B - V) = 5.8 \times 10^{21}$ atom cm^{-2} mag^{-1} (Bohlin, Savage & Drake 1978), where $N(H + H_2)$ is the column denisty, and $E(B - V)$ is the colour excess. In their calculation, they used the interstellar medium (ISM) gas-to-dust ratio. Meaburn & Lopez (1993) have observed also dusty globules of gas in the Dumbbell nebula (M27) with a lower density (n_H is $\sim 5.0 \times 10^4$ cm^{-3}) than those in the Helix nebula. The estimated densities of the clumps depend on the (uncertain) values of PN distances, and on the gas-to-dust ratio, which is unknown inside the clumps. In the present work we adopted a lower n_H value, consistent with that deduced in M27, because it has an accurate distance estimate (Meaburn & Lopez 1993).

At the early stages where the PN shells are still compressed and close to the central star, the temperature and density in the ionized and neutral shells are high. These two parameters decrease gradually as the PN shells expand and sweep away from the central star. At the same time, the incident flux of ultraviolet (UV) radiation decreases from $\sim 10^5$ times that of the ISM in the early stage, to 10–100 times that of the ISM at the late stage.

Bachiller et al. (1997) reported that the clumps which form the envelopes of the evolved PNe maintain high densities (a few times 10^5 cm^{-3}) and low temperatures ($\sim$25 K) from multi-line observations of CN, CO, and HCO^+. Their observations, of a sample of seven objects at different stages of development, showed that there are clear trends in the chemical evolution of the molecular envelopes. As a star evolves beyond the AGB, through the proto-PN and PN phases, the abundances of SiO, SiC_2, CS and HC_3N decrease, such that they are not detected in the PNe, while the abundances of CN, HCN, HNC and HCO^+ increase dramatically.

The clumping of the gas in the neutral envelopes of PNe is an essential aspect of both physical and chemical evolution. It

★E-mail: Tom.Millar@umist.ac.uk

represents the environment needed for the survival of the molecular gas, especially during the transition from the AGB stage to the early phase of PNe. This transition stage is dominated by high temperature owing to the effects of shocks.

The pioneering work in modelling the neutral shell of PNe was done by Black (1978). He modelled the transition zones of ionized PNe, and predicted the presence of simple molecules, like H_2, H_2^+, HeH^+, OH and CH^+. Howe, Millar & Williams (1992) have modelled the chemical evolution of clumps, such as those observed in the Helix nebula, during the transition from the red giant phase to PNe phase. They found that the reformation of molecules in the shocked gas leads to the synthesis of small molecules and ions such as CH, CH_2, and CH_3^+. The shocks are more likely to play a role in the early evolutionary stages, especially the proto-PN phase, when stellar winds compress and heat the inner surface of the molecular envelope (Cox 1997). Therefore we exclude the effect of shocks in the treatment of our models for evolved PNe. A steady-state chemical model has been constructed by Howe, Hartquist & Williams (1994). The estimated CN/HCN ratio is comparable to the observed ratio, while the HNC/HCN ratio predicted by their model is a factor of 20 lower than observed and the HCO^+ abundance about 3 orders of magnitude lower than that observed.

Based on recent extensive observations of the early type PN NGC 7027 by the *Infrared Space Observatory* (*ISO*), Yan et al.(1999) present a thermal–chemical model of the neutral envelope of NGC 7027. Also very recently, Hasegawa, Volk & Kwok (2000) have developed a spherically symmetric, steady-state chemical model for NGC 7027. Their predicted CN/HCN ratio is about 30 throughout the wind region and 1–10 in the dense shell, comparable to the observed values in PNe.

The objective of the current paper is to use a detailed time-dependent chemical model to investigate the chemistry of clumpy neutral envelopes of the three nebulae NGC 6781, M4-9 and NGC 7293. Our motivation is based on recent published observed molecular abundances in these PNe in addition to improvements in the UMIST chemical network data base. A study of the neutral envelopes of the early-type PNe is the topic of future work.

In Section 2, we present the initial parameters of the models and the chemical network. Section 3 shows the results and contains a discussion of the different models. Conclusions are given in Section 4.

2 GAS-PHASE MODELS

2.1 Initial parameters

We have constructed three models: model M1 for NGC 6781, M2 for M4-9, and M3 for NGC 7293. The initial fixed parameters of these models are summarized in Table 1. The density, temperature and UV radiation values are roughly those observed in the clumps of evolved PNe (Bachiller et al. 1997). We have considered models with various values for the cosmic ray ionization rate, with enhancement factors of 1–10^4 over the interstellar value of $1.3\times10^{-17}\,s^{-1}$. Enhancements greater than 1 simulate the large ionization rates that can be produced by X-rays. X-ray ionization differs from that produced by cosmic rays and UV photons in that it can produce multiply charged ions, such as C^{++}, and ionize elements with high ionization potentials, such as O and N. However, ions so produced undergo rapid charge exchange reactions and transfer their ionization to H^+ and H_2^+, and thence to H_3^+, which are the dominant ions produced by cosmic rays. We have investigated varying the initial abundances but find that, for reasonable variations, the observed abundances can be fitted by a consistent set of values but at different times. In this sense, our study investigates the evolutionary differences between the three models M1, M2 and M3.

Table 1. Initial values for model parameters.

Parameters	Values
Temperature (K)	15
Density (cm^{-3})	4×10^4
Visual extinction (A_V)	1.0
UV enhancement	10
CR enhancement	10^4

Table 2. Initial elemental abundances relative to total hydrogen.

Element	Abundance	Element	Abundance
H	0.1	S	1×10^{-6}
H_2	0.45	Si	1×10^{-6}
He	0.13	Mg	1×10^{-6}
C	5×10^{-4}	Na	1×10^{-6}
N	See text	Cl	1×10^{-6}
O	3.3×10^{-4}	Fe	1×10^{-6}

2.2 The chemical network

We have used the chemical reaction network and rate coefficients (complete RATE 95 data base) of Millar, Farquhar & Willacy (1997). The chemical network in our models has 3893 reactions and 397 species. The observed molecular species in envelopes around AGB stars (Olofsson 1997) are taken as initial molecular abundances for our calculations. The value for n_C/n (where n is the total number density of hydrogen) was assumed to be 5×10^{-4}, slightly larger than that in the ISM when account is taken of the presence of some carbon (and oxygen) in dust grains. The clumps are treated as carbon-rich ($n_C/n_O > 1$) clumps with $n_C/n_O = 1.5$. The elemental abundances for metals (i.e S, Si, Mg, Fe, Na) are adopted with their high ISM observed values, because the physical conditions inside the clumps are roughly similar to that found in molecular clouds. The adopted value for n_{He}/n is 0.13, consistent with the abundance ratios recommended by Clegg (1987). The initial abundance of atomic hydrogen is assumed to be 10 per cent of the total hydrogen density. Table 2 gives the initial elemental abundances relative to total hydrogen nuclei. They are fixed in this study except that for nitrogen. It varies for each source, with $n_N/n_O = 0.4$ (NGC 7293), 0.51 (NGC 6781), both from Bachiller et al. (1997), and 0.45 (M4-9).

3 RESULTS AND DISCUSSION

In Fig. 1, we plot the calculated abundances of CN, HCN, HNC and HCO^+ relative to ^{13}CO versus the ionization in units of the ISM rate. The ultraviolet radiation field, in units of the Habing field, temperature, interstellar extinction and density are given in Table 1. The abundances of CN, HCN, HNC and HCO^+ barely increase with enhancement factor in the range 1–100. There is gradual

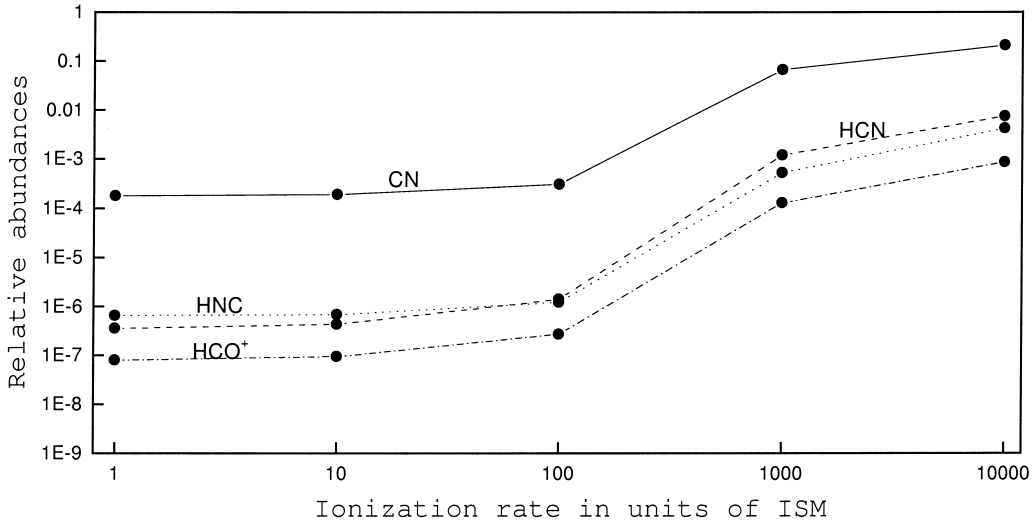

Figure 1. The calculated abundances at 10^4 yr, relative to ^{13}CO, are plotted versus the ionization rates, in units of the average ISM rate. Solid, dashed, dotted and dot–dashed lines represent CN, HCN, HNC and HCO^+ respectively. The calculated abundances increase with the ionization rate. At an enhancement of 10 000, HCN, HNC and CN abundances match well to the observed values, while HCO^+ is about half an order of magnitude less than observed.

increase of the abundances of the different species as the enhancement increases above 100, as the effects of ionization begin to dominate over photoeffects. We note that photons produce C^+ as the major ion, whereas cosmic rays produce H_3^+ and related molecular ions. One can envisage the change in molecular abundances as the ionization by cosmic rays increases as being similar to the change that occurs as one moves from diffuse to dense molecular clouds, from material dominated by photons to that dominated by cosmic rays. The abundances of HCN, and HNC are in good agreement with the observations at an enhancement of 10 000, while HCO^+ is about a factor of 3–5 less. The results of Fig. 1 correspond to a time taken to be 10^4 yr, the average age deduced from our three model calculations. These results show that the high ionization rate is important in reproducing the observed abundances, particularly that of HCO^+. We have tested a model using the standard ISM ionization rate with higher values of $A_V \geq 3.5$. The results of the model show a poor fit with observational values of CN, HCN and HNC, while the calculated abundance of HCO^+ in this case was less than the observation by four orders of magnitude.

Based on Fig. 1, we present the detailed results from one chemical model applied to these three evolved PNe. The model is characterized by a high rate of ionization, which can be attributed to a high cosmic ray ionization rate plus soft X-rays from the hot central star. X-ray observations for several PNe have been reported earlier by Apparao & Tarafdar (1989). Their observations strengthen the conclusion that the X-rays emanate from the central star and not from the nebula. Such a large ionization rate seems to be needed given the large abundance of HCO^+ observed in evolved PNe (Deguchi et al. 1990; Bachiller et al. 1997). The UV radiation field from the central star is assumed to be 10 times that of the ISM.

We have calculated a time-dependent model for comparison with observation and adopt an evolutionary age of 8000, 10 000, and 12 000 yr for NGC 6781, M4-9 and NGC 7293, respectively. These times represent the dynamical ages of each of these objects, where the dynamical age is calculated using the linear radius and expansion velocity of the object. The dynamical age of a PN depends on the distance estimation, which is somewhat uncertain.

The calculated abundances relative to ^{13}CO for NGC 6781, M4-9 and NGC 7293 are given in Tables 3–5 respectively. In column 1, we give the name of molecular species, column 2 shows the observed abundances relative to ^{13}CO, and column 3 shows the calculated abundances relative to ^{13}CO for every object. The calculated abundances of all three models show reasonable agreement with observations. The molecular species HCN, HNC, HC_3N and SiC_2 are in good agreement with observational values, although the latter two species have only upper limits, while CN is

Table 3. The calculated abundances of species relative to ^{13}CO in NGC 6781 at a time of 8000 yr.

Species	Obs.[1]	M1
^{12}CO	20	20
CN	1.2×10^{-1}	2.5×10^{-1}
HCN	1.0×10^{-2}	9.5×10^{-3}
HNC	7.0×10^{-3}	5.3×10^{-3}
HCO^+	8.0×10^{-3}	9.7×10^{-4}
CS	$<1.1\times10^{-3}$	6.5×10^{-3}
HC_3N	$<2.0\times10^{-3}$	8.3×10^{-8}
SiO	$<4.0\times10^{-4}$	1.5×10^{-3}
SiC_2	$<1.3\times10^{-3}$	1.0×10^{-4}

[1]Bachiller et al. (1997)

Table 4. The calculated abundances of species relative to ^{13}CO in M4-9 at a time of 10 000 yr.

Species	Obs.[1]	M2
^{12}CO	18	18
CN	8.5×10^{-2}	2.1×10^{-1}
HCN	9.0×10^{-3}	7.5×10^{-3}
HNC	2.0×10^{-3}	4.2×10^{-3}
HCO^+	3.0×10^{-3}	8.6×10^{-4}
CS	$<8.0\times10^{-4}$	5.3×10^{-3}
HC_3N	$<1.4\times10^{-3}$	5.9×10^{-8}
SiO	$<3.0\times10^{-4}$	1.3×10^{-3}
SiC_2	$<2.0\times10^{-3}$	8.4×10^{-5}

[1]Bachiller et al. (1997)

Table 5. The calculated abundances of species relative to ^{13}CO in NGC 7293 at a time of 12 000 yr.

Species	Obs.	M3
^{12}CO	9.3	9.3
CN	3.3×10^{-2}	9.8×10^{-2}
HCN	5.0×10^{-3}	3.4×10^{-3}
HNC	3.0×10^{-3}	1.9×10^{-3}
HCO^+	2.0×10^{-3}	4.4×10^{-4}
CS	$<3.0\times10^{-3}$	2.4×10^{-3}
HC_3N	$<7.0\times10^{-4}$	2.4×10^{-8}
SiO	$<3.0\times10^{-4}$	6.4×10^{-4}
SiC_2	$<9.0\times10^{-4}$	3.9×10^{-5}

[1]Bachiller et al. (1997)

Table 6. Averaged abundance ratios in evolved planetary nebulae.

	Obs.[1]	Model
CN/HCN	9	~28
HNC/HCN	0.5	~0.5
HCO^+/HCN	0.5	~0.1

[1]Bachiller et al. (1997)

Table 7. Abundances of selected species relative to ^{13}CO.

Species	M2
CH	9.9×10^{-1}
CH_2	3.7×10^{-2}
CH_3	4.7×10^{-3}
C_2H	5.4×10^{-2}
CH_2^+	9.6×10^{-3}
CH_3^+	1.6×10^{-3}
OH	3.5
H_2O	4.8×10^{-1}
HCl	5.1×10^{-2}

roughly 2–3 times the observed values and HCO^+ is about 3–8 less abundant.

The formation route of HCN, HNC and CN is as follows:

$$C^+ \xrightarrow{NH} CN^+ \xrightarrow{H_2} HCN^+ \xrightarrow{H_2} HCNH^+ \xrightarrow{e} HCN \text{ or } HNC \xrightarrow{h\nu} CN.$$

From Fig. 1 and the above route one can see that the parent molecular ion $HCNH^+$ is the main source for the formation of HCN, HNC and CN. With increasing the ionization rate, $HCNH^+$ increases, hence the daughter molecules increase.

The ionic species HCO^+ is formed by the route

$$H_2CO \xrightarrow{h\nu} CO \xrightarrow{CR} CO^+ \xrightarrow{H_2} HCO^+,$$

and destroyed by dissociative recombination with electrons. The observed abundances of CS and SiO are upper limits only. Our calculations give abundances close to, or sometimes in excess of, these upper limits, which may indicate that sulphur and silicon are depleted to a greater extent than adopted here.

In Table 6, we compare the calculated averaged abundance ratios of CN, HNC, and HCO^+ relative to HCN with the observed values. The CN/HCN ratio is roughly three times the observed average abundance ratio, while HNC/HCN is similar to that observed. The HCO^+/HCN ratio is about one fifth of the observed ratio. From Table 6, it appears that our results, in general, are improved over those found by Howe et al. (1994), whose estimated CN/HCN ratio is about 10 times the observed ratio, while their HNC/HCN ratio is a factor of 20 lower and their HCO^+ abundance about 3 orders of magnitude lower than those observed. This is mainly a result of the following differences between our models and that of Howe et al. (1994): (i) the cosmic ray ionization rate we have used is 10^4 times the rate they used; (ii) we adopted the AGB initial molecular abundances, while they started from atoms and atomic ions, except for H_2; (iii) we used a more recent reaction rate file (Millar et al. 1997); and (iv) we used time-dependent models, while they used steady-state models.

Table 7 shows high abundances of some unobserved species. The model predicts that OH and H_2O are abundant even in these carbon-rich environments. These results are consistent with the detection of these two species in the young PN NGC 7027 by *ISO* (Liu et al 1996). However the production of OH, H_2O and hydrocarbon molecules in our models does not require hot chemistry such as that of NGC 7027. The water molecule is formed via

$$H_2 \xrightarrow{CR} H_2^+ \xrightarrow{H_2} H_3^+ \xrightarrow{O} OH^+ \xrightarrow{H_2} H_2O^+ \xrightarrow{H_2} H_3O^+ \xrightarrow{e} H_2O,$$

while OH is mainly formed through H_2O photodissociation. The molecules CH, CH_2, CH_3, C_2H, CH_2^+, CH_3^+ and HCl may be detectable in evolved PNe if the clumps are carbon-rich, although the HCl abundance depends directly on the elemental abundance of chlorine adopted and could be smaller than calculated here. Hasegawa et al. (2000) also predict the presence of the small hydrocarbon species, CH_2 and CH_3, in the young PN NGC 7027.

The routes predicted in our models for hydrocarbon (CH, CH_2, CH_3 and CH_4) formation are essentially initiated by the radiative association of C^+ with H_2:

$$C^+ \xrightarrow{H_2} CH_2^+ \xrightarrow{H_2} CH_3^+ \xrightarrow{H_2} CH_5^+ \xrightarrow{e} \ldots$$

$$\ldots \xrightarrow{e} CH_4 \xrightarrow{h\nu} CH_3 \xrightarrow{h\nu} CH_2 \xrightarrow{h\nu} CH$$

$$\downarrow$$

$$CH_2 \xrightarrow{h\nu} CH,$$

where the photodissociation of CH_4 can give both CH_3 and CH_2.

The HCl molecule is formed by

$$Cl \xrightarrow{h\nu} Cl^+ \xrightarrow{H_2} H_2Cl^+ \xrightarrow{e} HCl.$$

4 CONCLUSIONS

We have studied the pesudo-time-dependent chemical evolution of dense clumps in PNe. The high abundance of HCO^+ in PNe can be explained in terms of a high ionization rate, enhanced by a factor of about 10^4 above the ISM value, most likely because of X-ray emission from the hot central star.

Compared with observations, the calculated fractional abundance of CN is too large by a factor of 2–3, and HCO^+ is less abundant by about a factor of 5. Our models predict too much CS and SiO, although they are dependent on the elemental depletions adopted for sulphur and silicon. The HCN, HNC, HC_3N and SiC_2 abundances are in good agreement with the observations. The

models show that molecular species such as CH, CH_2, CH_3, C_2H, CH_2^+, CH_3^+, HCl, OH and H_2O are likely to be abundant in these objects.

ACKNOWLEDGMENTS

The authors are most grateful to the referee for valuable comments. Astrophysics at UMIST is supported by a grant from PPARC. This collaboration has been sponsored in part by the British Council, who provided support for TJM's visit to the Department of Astronomy, Cairo University. OMS acknowledges the support of his visit to Seoul National University by the BK-21 Korean program for Science Foundation.

REFERENCES

Apparao K. M. V., Tarafdar S. P., 1989, ApJ, 344, 826
Bachiller R., Planesas P., Martin-Pintado J., Bujarrabal V., Tafalla M., 1989a, A&A, 210, 336
Bachiller R., Bujarrabal V., Martin-Pintado J., Gomez-Gonzalez J., 1989b, A&A, 218, 252
Bachiller R., Huggins P. J., Cox P., Forveille T., 1993, A&A, 267, 177
Bachiller R., Forveille T., Huggins P. J., Cox P., 1997, A&A, 324, 1123
Black J. H., 1978, ApJ, 222, 125
Bohlin R. C., Savage B. D., Drake J. F., 1978, ApJ, 224, 132
Clegg R. E. S., 1987, in Torres-Peimbert S., ed., Proc. IAU Symp. 131, Planetary Nebulae. Kluwer, Dordrecht, p. 139
Cox P., 1997, in van Dishoeck E. F., ed., IAU Symp. 178, Molecules in Astrophysics: Probes and Processes. Kluwer, Dordecht, p. 477
Deguchi S., Izumiura H., Kaifu N., Mao X., Nguyen-Q-Rieu, Ukita N., 1990, ApJ, 351, 522
Hasegawa T. I., Volk K., Kwok S., 2000, ApJ, 532, 994
Howe D. A., Millar T. J., Williams D. A., 1992, MNRAS, 257, 419
Howe D. A., Hartquist T. W., Williams D. A., 1994, MNRAS, 271, 811
Kastner J. H., Weintraub D. A., Gatley I., Merrill K. M., Probst R. G., 1996, ApJ, 462, 777
Liu X.-W. et al., 1996, A&A, 315, L257
Meaburn J., Lopez J. A., 1993, MNRAS, 263, 890
Meaburn J., Walsh J. R., Clegg R. E. S., Walton N. A., Taylor D., Berry D. S., 1992, MNRAS, 255, 177
Millar T. J., Farquhar P. R. A., Willacy K., 1997, A&AS, 121, 139
Olofsson H., 1997, Ap&SS, 251, 31
Yan M., Federman S., Dalgarno A., Bjorkman J. E., 1999, ApJ, 515, 640

This paper has been typeset from a TEX/LATEX file prepared by the author.