Physics and chemistry of the late stages of stellar evolution – an introduction

Sun Kwok

Laboratory for Space Research, Faculty of Science, The University of Hong Kong, Hong Kong, China
E-mail: sunkwok@hku.hk

Abstract. The stellar evolution from the asymptotic giant branch (AGB) to planetary nebulae (PN) contains some of the most interesting physical and chemical processes in the Universe. Within a time period of one million years starting from the nucleosynthesis of carbon in the core, we witness the chemical synthesis of molecules in the atmosphere, followed by the condensation of minerals and organics in the stellar outflow. Different phases of supersonic stellar winds, both spherical symmetric and highly collimated, and their interactions lead to a series of dynamical processes and morphological transformation of the stellar ejecta.

Most interestingly, PN are now known to be major sources of complex organics in the Galaxy. Organic compounds of mixed aromatic and aliphatic structures have been observed to form in the post-AGB evolution over time scales as short as hundreds of years. There is likely that these stellar organics journeyed through the Galaxy and were embedded in early Solar System.

1. Introduction
The asymptotic giant branch (AGB) phase of stellar evolution is characterized by two major events: one is the nucleosynthesis of the chemical element carbon (C) by helium (He)-shell burning above the core, and the other is the initiation of a strong stellar wind at the surface. Through convection, C is dredged up from the core to the envelope. As the star ascends the AGB, the envelope expands, the luminosity increases, and the surface temperature drops. When the surface temperature falls to below 3000 K, simple molecules begin to form in the photosphere and solid-state materials condense in the extended atmosphere. Radiation pressure on the solid grains drags the gas along, resulting in large-scale mass loss of the stellar envelope. Such mass loss is capable of completely depleting the hydrogen (H) envelope. The exposure of the hot core and the subsequent initiation of another phase of high-speed mass loss results in dynamical wind interactions. The rapidly evolving hot core gradually photo-ionize the circumstellar medium, creating the spectacular phenomenon of planetary nebulae (PN)[1]. At the same time, chemical synthesis of increasingly complex molecules and solids occurs in the circumstellar environment, cumulating in the formation of complex organics. In this paper, we review the rich physical and chemical processes at play during the AGB-PN evolution.

2. Mass loss on the AGB
Large-scale mass loss from AGB stars was discovered as the result of the detection of infrared excesses in the spectra of AGB stars [2]. Analysis of the double-peaked OH maser and CO
Figure 1. The extent of mass loss is illustrated in the spectral energy distribution of the extreme carbon star IRAS 21318+5631 where the stellar photosphere is completely obscured by its own ejected circumstellar dust envelope. The central star suffers from 360 magnitudes of extinction in the visible (A_V), and is undetectable in the optical region. Its infrared spectrum (solid green line) is due to dust emission and has a color temperature of 300 K. The dotted line represents the theoretical fit to the spectrum based on a 1-D radiation transfer model with a hidden 2500 K central star (dashed line) as the energy source. The absorption feature near the peak of the spectrum is the 13.7 µm band of acetylene.

thermal emissions suggests that these molecular phenomena are manifestations of a steady, low-velocity (∼10 km s^{-1}) stellar wind [3, 4]. The mechanism of mass loss was identified as radiation pressure on solid-state dust grains and the subsequent transfer of momentum from dust to gas through dust-gas collisions [5, 6]. The rates of mass loss can be estimated by both molecular-line and infrared observations. The mass loss rate steadily increases as the star ascends the AGB, from ∼10^{-7} M_☉ yr^{-1} during the early AGB to as high as 10^{-4} M_☉ yr^{-1} at the tip of the AGB. At the end of the AGB, the mass loss rate can be so high that the photosphere of the star is completely obscured by circumstellar dust and the star appears only as an infrared object [7] (Fig. 1). Such mass loss has significant effect on stellar evolution as it allows stars with initial mass as high as 8 M_☉ to evolve through the PN phase to white dwarfs without undergoing supernova explosions [8].

3. Effects of mass loss on the formation of planetary nebulae

While PN were commonly thought to be the result of sudden ejection of the H envelope of their parent stars, the discovery of mass loss on the AGB let us to the idea that the remnant of circumstellar envelopes ejected during the AGB phase must have an effect on the formation of PN. When the H envelope is completely depleted by mass loss and the core is exposed, the star will become hotter and bluer and the AGB wind ceases. A subsequent phase of less massive but faster mass loss, probably driven by radiation pressure on ionized gas, can compress and accelerate the remnant of the AGB wind to form the shell structure observed in PN [9]. If the interaction of the two winds is energy-conserving, then the expansion of the PN shell is driven by thermal pressure from the shocked fast wind [10].
Soon after the proposal of the interacting winds theory, the hypothesized fast winds from the central stars of PN were discovered by the newly launched International Ultraviolet Explorer (IUE) satellite [11]. In the following decade, development of CCD imaging technology made possible the detection of faint outer haloes of PN, therefore confirming the presence of AGB envelopes in PN [12, 13]. The AGB envelopes were also detected by infrared continuum observations by the Infrared Astronomical Satellite (IRAS) [14] and millimeter-wave observations of molecular lines [15]. Evidence for the shocked fast wind was found by diffuse X-ray continuum emission by the ROAST and Chandra satellites.

The detection of neutral materials in PN suggests that PN contain more than just ionized gas, but also molecular and solid-state components as well. The amount of mass contained in the molecular component is much higher than in the ionized gas component and can play a role in the morphological transformation of PN (see section 5). The chemical constituents of the neutral matter also led to the use of PN as chemical laboratories (see section 8).

4. Morphological structure of planetary nebulae

High dynamic-range CCD imaging observations of PN show that PN have complex morphological structures. In addition to the high-density shell, there are also rims, crowns, and haloes [16]. At the same time, the central star is evolving rapidly to high temperatures, at a rate that is highly dependent on its mass [17]. The rapid change in temperature of the central star results in a hardening of radiation emitted by the central star and a changing ionization structure of the circumstellar material. The observed multiple-shell structures of PN can only be understood by a consistent treatment of dynamics of interacting stellar winds coupled with stellar evolution (see Schönbener, these proceedings).

5. Stellar metamorphosis

While the 1-D dynamical models can successfully explain the morphological structure of spherically symmetric PN, there exist many PN which have clear bipolar structures. Even some very well-known PN such as the Ring, the Helix, and the Dumbbell are likely to be bipolar systems viewed near pole-on. When one takes into account of projection effects, the fraction of bipolar nebulae is actually very high. The discovery and imaging of proto-planetary nebulae (PPN) shows that the transformation of the PN morphology occurs early, during the short (10^3 yr) transition from the end of the AGB to the PN stage [18]. The mechanism of shaping is still not understood, although time-dependent outflows collimated by an equatorial torus probably play a role.

PN are optically bright because of the strengths of the recombination lines of H and He and collisionally excited lines of metals. As a result, our view of PN are highly biased by their optical images. The amount of ionized mass in PN are typically 10^{-2} – 10^{-1} M_\odot, but the amount of molecular mass can be 10 to 100 times higher. It would be desirable to directly map the structure of the neutral matter. This can be done by molecular-line and far-infrared imaging observations. Submillimeter-wave imaging observations have resulted in the detection of the molecular torus [21] and imaging observations by the Spitzer satellite has found evidence of cold dust beyond the optical nebula [22]. Indirectly, the tight waists seen in bipolar nebulae such as NGC 6302 and NGC 2346 is evidence that these PN are confined by an unseen external medium. The optical lobes therefore do not represent where the majority of masses reside, but cavities cleared out by collimated outflows [19]. In the case of PPN, the bright optical lobes are the result of illumination effects [20].

High dynamic-range imaging observations have resulted in the detection of an increasing numbers of PN with multipolar structures [23, 24]. It is possible that multipolar structures are very common as many of the observed morphologies of PN can be explained by a universal multipolar model of PN [25]. While multipolar PN can have several pairs of bipolar lobes oriented
at different directions, they are usually of similar physical lengths when projection effects are taken into account. These are therefore unlikely to represent masses ejected by separate events, but instead are evacuated cavities in the neutral envelope cleared out by high-speed outflows leaked out from holes in the torus.

Although we have made a lot of progress in understanding the physical origin of the morphological structure of PN through the interacting winds model, there are still many unsolved questions. The fast outflows can be directional, or even time dependent. The physical mechanism of collimation is not understood. Future observations of higher sensitivity and dynamic range (e.g., by ALMA and SOFIA) are needed to map out the distribution of neutral matter outside of the ionized nebulae for us to have a complete picture of the structure of PN.

6. Symbiotic stars, novae and binary evolution
When an AGB star is a member of a binary system, its stellar wind can be accreted onto the main sequence companion, resulting in the symbiotic phenomenon. If the companion has a higher initial mass and has already evolved through the PN stage to become a white dwarf (WD), then the wind accretion could result in the ignition of H burning on the WD, creating a symbiotic nova. The most famous examples of this class are V1016 Cyg and HM Sge. If the accretion rate is high, the WD can even evolve backwards to the red, leading to the born-again phenomenon [26]. For an AGB-WD system, the WD can photoionize the AGB wind, resulting in a PN-like emission-line system. The WD can even have a high-speed wind, causing a colliding winds situation between the winds of the two components [27]. Morphologically, these binary systems can resemble the appearance of PN because many similar physical processes are at work. PN and symbiotic stars have to be distinguished not so much by their observational properties but their evolutionary status [28].

The declining light curve of classical novae is the result of shrinking photosphere and the re-ignited, H-shell-burning WD evolving to the blue at constant luminosity [29]. The radio and visible light curves of novae can be explained by a decreasing rate of mass loss after the outburst [30]. The fact that novae can change from a free-free dominated spectrum to a dust-emission dominated spectrum over a period of days is the best illustration that solids can form efficiently in an low-density environment.

7. Circumstellar synthesis of molecules and solids
Rotational transitions of over 80 molecules have been detected in the circumstellar envelopes of AGB stars and PN (see Cernicharo, these proceedings). The list of molecules include inorganics (CO, SiO, SiS, NH3, AlCl), organics (C2H2, CH4, H2CO, CH3CN), radicals (CN, C2H, C3, HCO+), rings (C3H2), and chains (HC9N). AGB stars are therefore prolific molecular factories. Infrared spectroscopic observations also found that solid minerals can condense in large quantities directly from the gas phase in the stellar wind. Over 4000 O-rich AGB stars are detected to show the 9.7 µm feature of amorphous silicates and 700 C-rich AGB stars to show the 11.3 µm SiC features [31]. Since the dynamical times scales of AGB envelopes, PPN, and PN are 10^4, 10^3, and 10^4 yr, respectively, we are actually witnessing chemical synthesis at work on these short time scales.

8. Circumstellar synthesis of complex organics
When the stars evolve from the AGB to PN, the chemical composition of the solid-state component changes significantly. While amorphous silicates, silicon carbide, and various refractory oxides dominate the spectra of AGB stars, a family of unidentified infrared emission (UIE) features emerges in PN [32]. These features were identified as vibrational modes of aromatic compounds [33]. Since the UIE features are not seen in the progenitor AGB stars, these organic compounds must have been synthesized in situ in the stellar outflow during the
short (∼10³ yr) PPN phase. Indeed, infrared spectroscopic observations of PPN show that the UIE features are already present in PPN [34]. In addition to the aromatic features, aliphatic features due to C–H stretches of CH₃ and CH₂ around 3.4 µm are also detected in PPN [35, 36]. Accompanying the UIE features are strong and broad emission plateau features around 8 and 12 µm, which are most likely due to superpositions of in-plane and out-of-plane bending modes of a variety of aliphatic chains attached to the peripherals of aromatic rings [37].

9. Origin of the UIE features
The UIE phenomenon consists of aromatic features at 3.3, 6.2, 7.7, 8.6, and 11.3 µm, aliphatic features at 3.4 and 6.9 µm, weaker unidentified features at 15.8, 16.4, 17.4, 17.8, and 18.9 µm, and broad plateau features at 8, 12, and 17 µm. What is the chemical structure of the carrier of all these features? The most popular model is the polycyclic aromatic hydrocarbon (PAH) hypothesis, where the UIE features are the result of infrared fluorescence from small (∼50 C atoms) gas-phase PAH molecules being pumped by far-ultraviolet photons [38]. The strongest argument for the PAH hypothesis is that single-photon excitation of PAH molecules can account for the 12 µm excess emission observed in cirrus clouds in the diffuse interstellar medium by IRAS [39, 40].

However, the PAH hypothesis faces a number of problems. PAH molecules have well-defined sharp lines but the observed UIE features are broad. PAH molecules are primarily excited by UV with little absorption in the visible, but UIE features are seen in PPN and reflection nebulae with no UV radiation. Actually, the shapes and peak wavelengths of UIE features are independent of temperatures of exciting stars [41]. The strong and narrow expected electronic transitions of PAH in the UV are not seen in interstellar extinction curves [42]. No specific PAH molecules have been detected in spite of the fact that the vibrational and rotational frequencies are well known [43].

Chemists are also uncomfortable with the PAH hypothesis as “no PAH emission spectrum has been able to reproduce the UIE spectrum w.r.t. either band positions or relative intensities” [44, 45]. In order to fit the astronomical observations, the PAH model has to appeal to a mixture of PAH of different sizes, structures (compact, linear, branched) and ionization states, as well as artificial broad intrinsic line profiles. The PAH model is so flexible that it has been shown to be able to fit the observed spectra of silicates, hydrogenated aromatic carbon (HAC), coal, and even artificial spectra [46].

What are the alternatives to the PAH model for the carrier of the UIE features? By introducing H into graphite (sp²) and diamond (sp³), a variety of amorphous C-H alloys can be created. By varying the aromatic to aliphatic ratio, geometric structures of mixed hybridization states can be artificially produced. A variety of laboratory techniques involving injection of different forms of energy into a mixture of gas-phase hydrocarbons followed by condensations on substrates has resulted in many different forms of amorphous hydrocarbons [47, 48, 49, 50]. These artificial substances share common properties with natural substances such as coal [51], kerogen [52], petroleum [53], soot and other products of combustion [54] in that they consist of islands of aromatic rings linked by aliphatic chains of different lengths of orientations. The amorphous nature of these particles is demonstrated by X-ray diffraction studies [55]. Figure 2 shows a comparison between the laboratory spectrum of HAC to the astronomical UIE spectrum of a PN.

10. The MAON model
Spectral analysis of the spectra of PN shows that a significant fraction of the energy emitted in UIE features above the infrared continuum arise from the aliphatic component. This led us to propose that the carrier of the UIE features are best represented by mixed aromatic/aliphatic organic nanoparticles (MAON for short). These are complex organic solids with disorganized
structures consisting of small units of aromatic rings linked by aliphatic chains, including impurities of O, N, S. A typical nanoparticle may contain multiple of such structures with several hundred C atoms [56, 57]. MAON are different from PAH in that they are amorphous with no fixed structure, contains a mix of rings and chains, contain impurities, and are three dimensional in structure.

How do such complex organics form in the circumstellar environment? Some find it very difficult to accept that organic solids can condense directly from gas-phase molecules under near vacuum conditions. However, observationally we see aliphatics and aromatics form in PPN on time scales as short as hundreds of years. In novae, they are actually observed to form on a time scale of days or weeks [58].

11. Star and Solar System connection

The traditional picture of objects in the Solar System is that they are made of minerals, metals, and ices. In the past 30 years, there has been increasing evidence that organic molecules and solids are common in the Solar System, and they can be found in planets and their satellites, asteroids, comets, meteorites, and minor bodies in the outer Solar System. Interplanetary dust particles (IDP) show the 3.4 µm aliphatic feature similar to that seen in PPN [59]. Almost all biologically relevant organic compounds are present in the soluble component of carbonaceous meteorites [60]. Seventy percent of the organic matter in carbonaceous meteorites is in the form of insoluble organic matter (IOM), which chemical structure is similar to MAON [61]. Complex organics containing N, commonly referred to as tholins, are found in the surface of Titan [62]. The 3.4 µm features observed in the Titan atmosphere and comets have very similar profiles as those observed in PPN [63].

This raises the question on the origin of these organics: were they made in the solar nebula
or were they inherited from interstellar space? Since 95% of stars evolve through the AGB stage, a large quantity of complex organics is synthesized by stars and distributed throughout the Galaxy. The discovery of pre-solar grains in meteorites suggests that minerals produced by AGB stars can travel through the interstellar medium and end on the surface of the Earth. If stellar organics can also survive their journeys through the interstellar medium, it is quite possible that the early Solar System inherited some of these stellar organics [64].

12. Conclusions
The circumstellar envelopes of AGB stars and PN have provided us with excellent laboratories to study dynamical processes at work in the Galaxy. The lessons that we have learned from PN have been applied to Wolf-Rayet stars, supernovae, star-forming regions, and active galactic nuclei. Since PN are bright in all wavelengths across the electromagnetic spectrum from radio to X-ray, they can be studied with all the modern observational techniques in astronomy. Theoretical models of PN can be stringently tested by these multi-wavelength imaging and spectroscopic observations. The presence of all states of matter (ionized, atomic, molecular and solid-state) allows us to study the radiative interactions between all these components.

The circumstellar envelopes of AGB stars and PN also provide us with chemical laboratory to study chemical synthesis of molecules and solids in space. With the changing appearance and abundance of different species as stars evolve from AGB through PPN to PN, we have a direct view of chemical synthesis at work under a very low-density environment. The degree of complexity of the end products were totally unexpected and the observations creates great challenges to conventional theories. With the efficient synthesis of organics by stars, it is quite possible that stellar organics have enriched the entire Galaxy, and possibly even the early Solar System and the primordial Earth.

Recent research has demonstrated that the late stages of stellar evolution from the AGB to PN are important areas of study both from the physical and chemical points of view. It is even conceivable that the products of evolved stars could have implications on the biological evolution on Earth [65].

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