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On dust irradiation in planetary nebulae in the context of survivability of ices

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A R T I C L E I N F O

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A B S T R A C T

A large number of molecules are observed in planetary nebulae, including simple and, - the most common (H_2, CO and OH), more complex (H_2O, SiO, HCN, HNC, HCO^+), and even the polycyclic aromatic hydrocarbons and fullerenes containing a few dozen and more atoms. Water molecules are observed, as a rule, in the young objects, in the gas phase (water "fountains" and related water masers) and solid phase (emission of crystalline ice particles). On the other hand, the results of calculations by the Cloudy computer program, given in this paper, show that the abundance of water ice in planetary nebulae, other conditions being equal, depends on the ionization rate of hydrogen, which depends in turn on the flux of energetic particles (protons and alpha particles) in the range of MeV energies and higher. Calculated water ice column densities reach values of up to $10^{19} - 10^{20}$ cm^{-2} at the usual average ISM H_2 ionisation rate of 10^{-16} s^{-1} and sharply decrease at rates that are a thousand times larger. The possibility of an increased flux of energetic particles in planetary nebulae under conditions of the standard interacting stellar winds scenario is discussed, and it is concluded that the flux may locally exceed by 1–3 orders of magnitude that of galactic cosmic rays. This may have important implications for the chemistry of complex compounds under conditions of planetary nebulae, in particular, for models of the origin of fullerenes.

1. Introduction

To form planetary nebulae (PN) AGB stars need to have intense outflows at the transition phase to PN reviewed in details by Kwok (2000). Winds due to thermal pulses of AGB stars - with mass loss rates of $\sim 10^{-5} - 10^{-4} M_\odot$/yr and velocities of 10–20 km/s - form the material of future PNe. The characteristic time scales of these processes are such that the increased temperature of the star at the end of the AGB stage causes photoionization of the ejected shell and transformation to the PN. Transition to the final phase takes place in a relatively short period of a few 100 years. At the same time the slow and intensive outflow of cold stellar matter is transformed into a hot, fast but less intense stellar wind with the rate of $\sim 10^{-9} - 10^{-7}$ $M_\odot$/yr and a speed of $\sim V_* \sim 1400 - 5000$ km/s (Kwok, 2000). The further dynamical evolution of the PN is determined by the interaction of the new rapid outflow with the previous slow one, causing the expansion of the PN at a rate of 20–40 km/s and larger.

Interestingly, a large number of molecules is observed in PN (Bachiller et al., 1997; Kwok, 2000; Josselin and Bachiller, 2003; Kimura et al., 2012; Zhang, 2016 and references therein) despite the high excitation: in the ionized part (the H^+ region), the gas temperature is about and more than 10^4 K, due to a strong hard radiation from the central star - a white dwarf (Kwok, 2000), with effective temperatures of about $5 \cdot 10^4 - 2 \cdot 10^5$ K (Werner, 2012; Ziegler et al., 2012). As usual, the existence of the molecules is connected to the region behind the photoionization and photodissociation fronts separating the inner fully ionized part from the outer neutral and molecular envelopes first described theoretically by Black (1978). The presence of such envelopes follows from observational and theoretical data about PN and AGB stars. Indeed, the observed mass of the H^+ zone is of order of several $0.1 M_\odot$ and does not exceed $0.5 M_\odot$, while stellar evolution on the AGB star demands the total (the sum of ionized, neutral and molecular parts) PN mass to be of the order of one or more solar masses, up to 3–4 $M_\odot$ (Kimura et al., 2012). Clearly molecules are present in the PN because of self-shielding by sufficient amounts of molecular gas in the form of the simplest and most common species (H_2, CO and OH), more complex species (H_2O, SiO, HCN, HNC, HCO^+) (Kimura et al., 2012), and even polycyclic aromatic hydrocarbons (PAHs) and fullerenes containing several tens or more atoms (Otsuka et al., 2014). Molecules of H_2O are observed both in the gas phase (water "fountain" and related masers in young PN)

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(Gomez et al, 2015; Blanco et al., 2014; Miranda et al., 2010) and in the solid phase (emission from crystal water ice) (Barlow, 1998; Kemper et al., 2002; Cohen et al., 1999).

It will be the main purpose of this work to explore the circumstances under which UV and CR radiation of ices may play a role in their survivability.

It should be also added, that molecules responsible for the characteristic features of the observed spectra, may be partly associated with nebular condensations. As is known, they are observed in PN as small (milli)globules with sizes of $\sim 10^{15}-10^{16}$ cm and concentrations of $\sim 10^5-10^6$ cm^{-3}: for example, in the nearest NGC 7293 there are about 3500 of such objects (Kwok, 2000). Probably, they formed in the AGB-wind phase, as a result of the Parker magnetohydrodynamic instability (Hartquist and Dyson, 1997), and should be differentiated from other types of (gas-dynamic) instabilities developing at a relatively later stages of the PN evolution (Breitschwerdt and Kahn, 1990; Kahn and Breitschwerdt, 1990). In general, such irregularities are important observable characteristics of all stellar winds, and PN are the good example of their manifestation (Dyson et al., 1989; Hartquist and Dyson, 1991). Dyson et al., (1989) describe the condensations as cold (about 10 K), dense ($\sim 10^6 cm^{-3}$) and molecular, with masses of the order of 10^{-6} $M_\odot$ each, surviving over the full PN dynamical lifetime of $\sim 10^4$ years (Redman et al., 2003). This prediction was confirmed by direct observations of NGC 7293 with (milli)globules by O'Dell et al. (2005). On the other hand, the characteristic times of the mentioned instabilities in PN, possibly leading to the formation of clumps, is clearly less than time of the PN phase (Capriotti and Kendall, 2006). Also H_2 molecules begin to dominate quickly via formation from atomic hydrogen on the surface of dust grains, for a time of about $1.5 \cdot 10^9/n$ years (Dopita and Sutherland, 2001), then forming a gas component, effectively shielding the inner regions of the condensation from the hard UV radiation (it should be recalled that photodissociation of H_2 is realized through the dominant reaction channel with the interaction cross-section of $\sim 10^{-14}$ cm^2 (Dopita and Sutherland, 2001). Under such conditions, saturated compounds like water, ammonia and methane are also formed and condensed on the grain surfaces with the characteristic timescale of $3 \cdot 10^9/n$ years (Ehrenfreund and Charnley, 2000). In other words, in condensations ($n \sim 10^6$ cm^{-3}) icy mantles of dust particles must form in a few thousand years; e.g., the most abundant solid water with frozen other volatiles (CO, NH_3 etc.) form the ice mantles with thicknesses up to a few 0.1 μ that are about one order of magnitude larger than the initial size of the silicate and/or graphite dust cores of ~ 0.01 μ coming from the AGB phase cold wind. In fact, the mentioned freeze out timescale does not take into account non thermal desorption and probably the corresponding formula overestimates the formation time of ice mantles. On the other hand under mentioned conditions of young PN icy particles may be already present there coming from the cold AGB outflows and surviving as long as they are shielded from radiation. In any case, because the time of the H_2 formation is also relatively small (about 1.5 thousand years under young PN and milliglobules conditions as compared with the dynamical time of 10^4 years) one may choose in a first approximation, a stationary model to describe the young PN and milliglobules in terms of the balance between the formation and destruction of the most important molecules (and ices). Thus, icy mantles on dust particles (water, ammonia, methane, methanol, carbon monoxide, etc.) are possible in the young PN and even in the milliglobules regardless of the condensations origin. Such icy particles are protected from exposure to extreme UV radiation and from vaporization during the lifetime of the (young) PN and that of the milliglobules. At the same time, as is known, these ices should be irradiated by UV with wavelengths larger than 912 Å According to experimental data, the irradiation of mixture of ices like $H_2O : CH_3OH : NH_3 : CO$ by the UV radiation with a photon energy of about 10 eV (vacuum UV, below VUV), causes the formation of highly complex compounds containing, for example up to 22 carbon atoms (Cottin et al,. 2001). It is also possible to form amino acids, PAH, etc. The threshold dose of the accumulated energy to initiate radiation-chemical transformation is 25 eV/molecule (Cottin et al., 2001).

It is interesting to note that, in recent years, infrared observations, as already noted, registered PAH, and even fullerenes C_{60} and C_{70} in the spectra of several PN, including 11 out of 338 observed by *Spitzer* (Otsuka et al., 2014). These authors interpret their observations as follows: the most likely places of formation of such compounds are the outflows of cold carbon stars in the AGB phase transition to the PN, but little details are known. In particular, it is unclear whether they are present initially in AGB winds, but not observed, due to the lack of appropriate sources of excitation, or they form during the process of transition to a PN phase. There is a point of view that fullerenes are formed by the UV destruction of hydrogenated amorphous carbon (HAC) and/or the dehydrogenation of large PAH molecules in the early PN stages, when there is the intense UV irradiation (Scott et al., 1997; Otsuka et al., 2014; Zhen et al., 2014). The quantitative description of this hypothesis is not known (see, however, Berne and Tielens, 2012) but many experimental data are available. Nothing is known about quantitative characteristics of the effectiveness of joint UV and corpuscular irradiation of dust inside the condensations and behind the PN photo-dissociation front. In a recent article Kwok (2011) discussed the possibility of recycling of organic matter in the Galaxy, just in the context of origin of the stable complex species during the transition phase from the AGB winds to the PN, with the possible formation of carbon-containing compounds. One should stress, however, that a no less important factor in the problem of the primary origin of complex compounds is the survivability of more abundant, but less stable ices (e.g. water etc.) and/or their mixtures under PN conditions. This article is devoted to the influence of the UV and corpuscular radiation on the survival of ices under early PN conditions, behind the photodissociation front. First, the physical-chemical model of PNe (with detailed description of an internal radiation field) will be calculated (Section 2) and the possibility of the existence of ices will be analyzed (Section 3). Second, the dose rate (the amount of absorbed energy per molecule per unit time) by UV and corpuscular radiation will be calculated, in order to reveal the possible formation of complex chemical compounds (Section 4). Conclusions are summarized in Section 5.

2. Physical and chemical model: the radiation field radial distribution under PN conditions and resulting chemistry

To calculate the effect of the irradiation on the surface of dust grains, one must have a physical-chemical model of the nebula, and, especially, the spatial dependent radiation field in the PN influencing the abundances of ices. Solution of the problem is complicated by non-stationary processes of molecular-ice component in PN (Tielens, 1992; 2005). However, as noted above, for the particular cases of high concentrations of early PN and condensations ($n \geq 10^6$ cm^{-3}) it is possible to use the stationary model, when the characteristic time of formation and destruction of ices (∼1000 years) is less than the characteristic dynamic time of the PN phase (∼10,000 years). On the other hand, for early PN the dynamic time is also about 1000 years while destruction of water ice is practically absent when the dust temperature is less than 110 K (see below). Thus the stationery model must be a good first approximation but the non-stationarity also should be investigated which will be presented later elsewhere.

To solve the stationery problem one can use the model, first described by Ferland et al. (1998) and the corresponding