Modelling the warm H$_2$ infrared emission of the Helix nebula cometary knots

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ABSTRACT

Molecular hydrogen emission is commonly observed in planetary nebulae. Images taken in infrared H$_2$ emission lines show that at least part of the molecular emission is produced inside the ionized region. In the best studied case, the Helix nebula, the H$_2$ emission is produced inside cometary knots (CKs), comet-shaped structures believed to be clumps of dense neutral gas embedded within the ionized gas. Most of the H$_2$ emission of the CKs seems to be produced in a thin layer between the ionized diffuse gas and the neutral material of the knot, in a mini-photodissociation region (mini-PDR). However, PDR models published so far cannot fully explain all the characteristics of the H$_2$ emission of the CKs. In this work, we use the photoionization code AANGABA to study the H$_2$ emission of the CKs, particularly that produced in the interface H$^+$/H$^0$ of the knot, where a significant fraction of the H$_2$ 1–0 S(1) emission seems to be produced. Our results show that the production of molecular hydrogen in such a region may explain several characteristics of the observed emission, particularly the high excitation temperature of the H$_2$ infrared lines. We find that the temperature derived from H$_2$ observations, even of a single knot, will depend very strongly on the observed transitions, with much higher temperatures derived from excited levels. We also proposed that the separation between the H$_\alpha$ and [N II] peak emission observed in the images of CKs may be an effect of the distance of the knot from the star, since for knots farther from the central star the [N II] line is produced closer to the border of the CK than H$_\alpha$.

Key words: astrochemistry – circumstellar matter – ISM: molecules – planetary nebulae: individual: NGC 7293 – planetary nebulae: individual: Helix nebula – infrared: ISM.

1 INTRODUCTION

Planetary nebulae (PNe) are formed by the ejection of the outer layers of low- and intermediate-mass stars (1–8 M$_\odot$) in their final stages of evolution. The ejecta originate while the star is on the asymptotic giant branch (AGB). Afterwards, the rapidly heating star drives a molecular dissociation front and an ionization front, which eventually over-run the ejecta. The study of the composition and structure of PNe, in particular, the molecular gas (its location, distribution and physical conditions), can provide information about the earlier evolutionary stages (Davis et al. 2003; Volk et al. 2004), as well as on the physics of dissociation and ionization fronts (Henney et al. 2007).

Infrared (IR) emission of H$_2$ has been identified in more than 70 PNe (Hora et al. 1999; Sterling & Dinerstein 2008), primarily bipolar nebulae (Kastner et al. 1996). The precise location of the observed H$_2$ emission and the dominant excitation mechanism are still under debate (Hora et al. 1999; Likkel et al. 2006; Henney et al. 2007).

Analysis of observations and models of the H$_2$ IR line emission of PNe indicate that the emission is produced both within the neutral envelope and within the ionized region (Aleman & Gruenwald 2004, and references therein). Aleman & Gruenwald (2011) showed that, in cases of high-temperature central stars, a significant part of the H$_2$ emission can be produced by the diffuse gas in the H$^+$/H$^0$ transition region of PNe.
The Helix nebula (NGC 7293) is an evolved PN excited by a \( T_\star = 120000 \text{ K}, \ L_\star = 100 \ L_\odot \) central star (Henry et al. 1999). High-resolution images of this PN have shown that the \( \text{H}_2 \) emission arises from its large population of globules, the so-called cometary knots (CKs), embedded in the ionized gas (e.g. Matsuura et al. 2009). Many authors argue that CKs are largely responsible for the \( \text{H}_2 \) emission produced within the ionized region (Beckwith et al. 1978; Gussie & Pritchet 1988; Reay et al. 1988; Teilens 1993; Schild 1995; Speck et al. 2002; Matsuura et al. 2009).

CKs are structures that resemble comets, particularly in images taken in \( \text{H}_\alpha, \ [\text{N} \\text{ii}], \text{S}6583, \) and \( \text{H}_2 \) 1–0 S(1) lines. Knots and filamentary condensations are also seen in other PNe (O’Dell et al. 2002) in the transition region between the ionized and neutral H. In the Helix nebula, the bright cusp points towards the central star and the tail in the opposite direction, which can indicate that the excitation is connected with the central star. Analyses of the emission of these structures suggest that they are significantly denser than the gas around them. While the typical diffuse gas density is around \( 10^2–10^3 \, \text{cm}^{-3} \) (Kwok 2000; Osterbrock & Ferland 2006), in the CKs the density is around \( 10^4–10^5 \, \text{cm}^{-3} \) (Huggins et al. 1992; Meaburn et al. 1998; Matsuura et al. 2007). The origin of the CKs is still uncertain. They may be formed within the original wind of the progenitor star or by instabilities and fragmentation of the swept-up shell during the onset of the PN phase. Huggins & Frank (2006) show that the latter is better supported by the observed properties of the knots. Matsuura et al. (2009) suggest a possible origin within a spiral density wave in the wind caused by an orbiting companion.

There is no evidence that the \( \text{H}_2 \) emission in CKs is produced by shocks (Huggins et al. 2002; O’Dell et al. 2005; Matsuura et al. 2007, 2008). On the other hand, as mentioned above, the emission of the CKs seems to be linked to the central star radiation field (O’Dell et al. 2005, 2007). The \( \text{H}_2 \) emission is more intense in a thin layer in the surface of the CKs towards the central star. However, analysis based on traditional models of photodissociation regions (PDRs) were unable to reproduce the high excitation temperature of the \( \text{H}_2 \) emission (\( \sim 900 \text{K} \)) estimated from the observations (Huggins et al. 2002; O’Dell et al. 2007). Recently, Henney et al. (2007) showed that advection can cause the ionization and dissociation front to merge, leading to enhanced heating of the molecular gas and reproducing well the excitation temperatures of \( \text{H}_2 \). It is evident from the work of Henney et al. that the physical conditions in the interface between the ionized diffuse gas and the CK are of key importance for the \( \text{H}_2 \) IR emission. The high excitation temperature of the \( \text{H}_2 \) emission could be naturally explained if part of the \( \text{H}_2 \) emission is produced in the \( \text{H}^+\text{H}^\circ \) transition of the CK.

In the present paper, the ionized and partially ionized regions of CKs are modelled with the one-dimensional photoionization code AANGABA. Our aim is to study in more detail the \( \text{H}_2 \) emission in the \( \text{H}^+\text{H}^\circ \) interface of the CK. A grid of models is obtained to study how the \( \text{H}_2 \) IR emission depends on different interface density profiles, CK radius, distance from the ionizing source and dust-to-gas ratio. We compare the \( \text{H}_2 \) IR emission with the atomic emission. Our calculations also provide good estimates of the \( \text{H}_2 \) formation and destruction rates inside the CKs, which indicate how long the molecule may survive inside the CKs and whether it forms \textit{in situ} or may have survived the earlier evolutionary phase.

We use our models to study the CKs in the Helix nebula (NGC 7293). The Helix is one of the nearest PNe (219 pc), and high-resolution images resolved the structure of the CKs (O’Dell et al. 2004; Meixner et al. 2005; Hora et al. 2006; Matsuura et al. 2007, 2008, 2009). The detailed observations allow us to test the model.

Our models are described in Section 2. The results are discussed in Section 3, and conclusions are summarized in Section 4.

2 MODELS

In Section 2.1, a brief description of the photoionization code AANGABA is given. The parameters assumed for the Helix nebula model are discussed in Section 2.2. A description of how the CKs were simulated is given in Section 2.3.

2.1 General description of the code

The AANGABA code simulates the physical conditions inside a photoionized nebula, given the ionizing spectrum, as well as the characteristics and distribution of gas and dust (Gruenwald & Viegas 1992). Since the gas and dust temperatures and densities depend on each other, as well as on the position inside the nebula, the code makes iterative calculations across the nebula. The code begins the calculations at the inner border of the nebula and continues the calculation in steps in the outward direction. In each location, the physical conditions, for example the ion and molecular density, the electronic density and temperature, the dust temperature and continuum and line emission, are calculated. The calculation ends when the code reaches the limit chosen by the user (for example a given ionization degree, gas temperature, optical depth, etc.). Geometrical dilution and extinction of the radiation by gas and dust are taken into account. The transfer of the primary and diffuse radiation fields is treated in the outward-only approximation.

12 elements and their ions are included in the code: H, He, C, N, O, Mg, Ne, Si, S, Ar, Cl and Fe. The species \( \text{H}_2, \text{H}_2^+, \text{H}_3^+ \) and \( \text{H}^- \) are also included in the code (\( \text{H}_2 \) is not included because it is unstable; Bordas et al. 1990). The density of each ion of each species is calculated with the assumption of chemical and ionization equilibrium. The processes of ionization, recombination and charge exchange are taken into account in the equilibrium equations of the atomic species. For the H-bearing species, 40 reactions of formation and destruction are included in the chemical equilibrium equations (Aleman & Gruenwald 2004).

The population of the \( \text{H}_2 \) rovibrational levels of the three lowest electronic bound states is calculated by assuming statistical equilibrium, i.e. the total population rate of a level is equal to its total depopulation rate. For the electronic ground level, several excitation and de-excitation mechanisms (radiative and collisional), as well as the possibility that \( \text{H}_2 \) is produced or destroyed in any given level, are included. For upper electronic levels, only radiative electronic transitions between each upper state and the ground state are included, since this must be the dominant mechanism. The population of the \( \text{H}_2 \) rovibrational levels of the electronic ground state by radiative mechanisms occurs through two main routes: electric quadrupole transitions between the rovibrational levels, involving

\[ \text{H}_2 \rightarrow \text{H}_2^\circ \text{H}^+ \text{H}^\circ \text{transition of the CK.} \]

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IR photons, or electric dipole transitions to upper electronic states with subsequent decay to the ground state, involving ultraviolet (UV) photons (UV pumping). Collisions may also change the H$_2$ energy level. We included collisions of H$_2$ with the main components of the gas, i.e. H, H$^+$, He, H$_2$ and electrons. In this work we are interested in the lines produced by the rovibrational transitions of H$_2$, whose wavelengths are in the 0.28 µm to 6.2 mm range of the electromagnetic spectrum. More details about the calculation of the H$_2$ level population can be found in Aleman & Gruenwald (2011).

The gas temperature is calculated assuming thermal equilibrium, i.e. the total input of energy in the gas per unit time and volume is balanced by the total loss of energy per unit time and volume. Several mechanisms of gain and loss of energy by the gas due to atomic species, dust and H$_2$ are taken into account. The gas heating mechanisms are photoionization of atoms, atomic ions and H$_2$ by the primary and diffuse radiation; H$_2$ photodissociation (direct and two steps); H$_2$ formation on grain surfaces, by associative detachment and by charge exchange with H; H$_2$ collisional de-excitation; and photoelectric effect on dust surfaces. The cooling mechanisms are emission of collisionally excited lines; radiative and dielectronic atomic recombination; thermal collisional atomic ionization; free-free emission; collisional excitation of H$_2$; destruction of H$_2$ by charge exchange with H$^+$; H$_2$ collisional dissociation; and collision of gas-phase particles with dust grains. Models by Tielens & Hollenbach (1985) and Spaans & Meijerink (2005) indicate that other molecules become important contributors to the thermal balance if $A_1 > 3.5$. Since in our models $A_1 < 2.7$, we do not include molecules other than H$_2$ in the thermal equilibrium.

### 2.2 The Helix model

The parameters for the Helix nebula model are given in Table 1. We assume that the central star radiates as a blackbody with $T_\star = 120 000$ K and $L_\star = 100 L_\odot$ (Henry et al. 1999; O’Dell et al. 2007). The density of the diffuse gas is $n_\text{D} = 50$ cm$^{-3}$ (Meixner et al. 2005).

Elemental abundances were determined by Henry et al. (1999) for He, O, C, N, Ne, S and Ar, from Helix line emission observations and ionization correction factors (ICFs) obtained from photoionization models. The C/O ratio obtained by Henry et al. (1999) is 0.87. The detection of C-bearing molecules, such as H$_2$CO, c-C$_2$H$_2$ and C$_3$H$_4$, has been used to argue that the Helix may be in fact C rich (Tenenbaum et al. 2009). We ran some models with C-rich abundances, but we found that it does not affect our results for H$_2$ significantly, and will assume the Henry et al. (1999) abundances. For the remaining elements taken into account in the code, Mg, Si, Cl and Fe, we adopt the values from Stasińska & Tylenda (1986).

Speck et al. (2002) model the IR emission of Helix and found the dust-to-gas ratio $M_D/M_g = 10^{-3}$, which is an average value for PNe (Stasińska & Szczepańska 1999). Our models assume by default amorphous carbon grains with a 0.1-µm radius. We also did calculations with silicate dust, but we found (as also discussed in Aleman & Gruenwald 2004) that the choice of compound does not cause significant changes in the H$_2$ density.

We assume a distance of 219 pc (Harris et al. 2007; Benedict et al. 2009), obtained from measurements of the central star parallax.

#### 2.3 Simulating the cometary knots

The CKs are simulated as an increase in the density profile of the Helix nebula model at a given distance. We construct a grid of CK models with different core densities ($n_k$), density profiles, dust-to-gas ratios ($M_D/M_g$) and distances from the central star ($R_k$). We obtain models with $n_k$ between $10^2$ and $10^4$ cm$^{-3}$ (Huggins et al. 1992; Meaburn et al. 1998; Matsuura et al. 2007). We assume that the density profile has an increase from $n_0$ to $n_k$ over a given distance $\Delta R$. In the following discussions, we call this region the interface of the knot. The region where the density reaches the maximum value ($n_k$) is called the core. We study four types of density profiles: step function (hereafter type 1), linear (type 2), $r^2$ (type 3) and exponential (type 4). According to O’Dell & Handron (1996), the Helix CKs have $M_D/M_g$ between $7 \times 10^{-4}$ and $7 \times 10^{-2}$. We obtain models for $M_D/M_g$ of $10^{-3}$ and $10^{-2}$. In each model, the dust-to-gas ratio and the chemical composition are assumed the same for CKs and diffuse gas. The parameters of the CK models discussed in the present work are listed in Table 2.

The code starts the calculations in the inner border of the nebula and continues outwards along the radial direction. At a given distance ($R_k$), an increase in density simulates the CK. For the present work, we calculate models with $R_k = 130-500$ arcsec (see discussion in Section 3.1). We stop the calculations where the gas temperature, which decreases with distance from the central star, reaches 100 K. We define $\Delta R_f$ as the distance from the border of the knot to this point.

#### Table 1. Input parameters for the Helix model.

| Parameter | Value$^a$ |
|-----------|-----------|
| $T_\star$ | 120 000 K |
| $L_\star$ | 100 L$_\odot$ |
| $n_\text{D}$ | 50 cm$^{-3}$ |
| Dust material | Amorphous carbon |
| Grain radius | 0.1 µm |
| Distance | 219 pc |
| Element      | Abundances (relative to H, by number) |
| He          | $1.20 \times 10^{-1}$ |
| O           | $4.60 \times 10^{-4}$ |
| C           | $4.00 \times 10^{-4}$ |
| N           | $2.48 \times 10^{-4}$ |
| Ne          | $1.52 \times 10^{-4}$ |
| S           | $1.48 \times 10^{-6}$ |
| Ar          | $3.10 \times 10^{-6}$ |
| Mg          | $3.80 \times 10^{-7}$ |
| Si          | $3.50 \times 10^{-7}$ |
| Cl          | $3.20 \times 10^{-9}$ |
| Fe          | $4.70 \times 10^{-7}$ |

$^a$References are given in the text.

#### Table 2. Parameters of the CK models.

| Model | $R_k$ (arcsec) | $\Delta R$ (arcsec) | $n_k$ (cm$^{-3}$) | $M_D/M_g$ | Profile |
|-------|---------------|---------------------|-----------------|-----------|---------|
| K1    | 129           | 0.0                 | $10^3$          | $10^{-3}$ | 1       |
| K2    | 129           | 0.2                 | $10^3$          | $10^{-3}$ | 2       |
| K3    | 129           | 0.2                 | $10^3$          | $10^{-3}$ | 3       |
| K4    | 129           | 0.2                 | $10^3$          | $10^{-3}$ | 4       |
| K5    | 129           | 0.01                | $10^3$          | $10^{-3}$ | 4       |
| K6    | 129           | 0.5                 | $10^3$          | $10^{-3}$ | 4       |
| K7    | 129           | 0.2                 | $10^3$          | $10^{-3}$ | 4       |
| K8    | 129           | 0.2                 | $10^3$          | $10^{-3}$ | 4       |
| K9    | 210           | 0.2                 | $10^3$          | $10^{-2}$ | 4       |
| K10   | 383           | 0.2                 | $10^3$          | $10^{-3}$ | 4       |
| K11   | 450           | 0.2                 | $10^3$          | $10^{-3}$ | 4       |
| K12   | 501           | 0.2                 | $10^3$          | $10^{-3}$ | 4       |
An IDL routine was developed to simulate a three-dimensional CK, allowing the calculation of surface brightness of atomic and H$_2$ lines by the integration of the emissivity along the line of sight inside the CK. In this routine, the knot is assumed to have cylindrical symmetry, with a semispherical head pointing in the direction of the central star. The CK is assumed to be seen edge-on. We assume that the one-dimensional profile of the emissivity, which is calculated with AANGABA, is the same for every line along the direction parallel to the symmetry axis, starting from the border of the knot. This is a simple approximation to simulate a comet-shaped knot, but it allows us to obtain a reasonable estimate of the H$_2$ line surface brightness. It is not our intention to reproduce the precise image of a CK.

3 RESULTS

3.1 Diffuse gas in the Helix model

Fig. 1 shows results for the Helix model obtained with the parameters of Table 1. The gas temperature profile is given in the top panel, while the radial profiles of H$^0$, H$^+$, H$^-$, H$_2^0$ and H$_2^+$ densities are plotted in the middle panel. Emissivities of some lines are shown in the bottom panel. The model in the figure applies to the diffuse gas only: it does not include CKs. The gas density and the dust-to-gas ratio are assumed to be uniform and equal to, respectively, $n_D = 50$ cm$^{-3}$ and $M_D/M_g = 10^{-3}$.

In the Helix, CKs are detected at distances from the central star (projected on the sky plane) between 132 and 384 arcsec (Matsuura et al. 2009). This interval is indicated by the grey band in Fig. 1. The three-dimensional morphology must be taken into account to calculate the real distance. The morphology of the Helix was studied by Meaburn et al. (1998) and O’Dell et al. (2004). According to Meaburn et al. (1998), the Helix structure (where the CKs are) has a toroidal shape, contained within an angle of about 20$^\circ$ on both sides of the equatorial plane of the nebula. The symmetry axis is inclined at about 37$^\circ$ with respect to the line of sight. O’Dell et al. (2004) found a slightly different value to the inclination angle, 28$^\circ$ with respect to the line of sight. Taking this geometry into account, real distances must be greater than the projected distances. For example, a CK in a plane inclined by 37$^\circ$ from the line of sight could be up to 25 per cent farther from the central star than the projected distance. Even with this deprojection, the CKs are not much farther than 500 arcsec from the central star, i.e. mostly inside the region where hydrogen is ionized. Our model also supports that the CKs coexist with the ionized species He$^+$, N$^+$, N$^{++}$, O$^+$ and O$^{++}$ in the diffuse gas. Our model has parameters similar to those of model 135/315 of Henry et al. (1999) and provides similar results for the ionization structure.

According to Matsuura et al. (2009) and Meixner et al. (2005), the H$_2$ emission of the Helix is associated with the CKs, although the instrumental resolution cannot exclude a contribution from the diffuse gas in the outer ring. As can be seen in Fig. 1, the calculated H$_2$ 1–0 S(1) emissivity from the diffuse gas is very low. Assuming a spherical gas distribution, the maximum H$_2$ 1–0 S(1) intensity is $10^{-8}$ erg cm$^{-2}$ s$^{-1}$ sr$^{-1}$, and the total 1–0 S(1) flux coming from inside the ionized region is $4 \times 10^{-13}$ erg cm$^{-2}$ s$^{-1}$. In contrast, the observed 1–0 S(1) flux of the Helix nebula is about $2 \times 10^{-9}$ erg cm$^{-2}$ s$^{-1}$ (obtained from the observations published in Speck et al. 2003). The flux obtained with our model without CKs shows that the diffuse ionized gas contributes less than 0.02 per cent of the observed emission. Our calculation of the flux above does not take into account a possible increase in the average gas density in the rings or the shielding of the radiation by the CKs, which may increase the H$_2$ emission.

3.2 Physical and chemical properties of CKs

Figs 2–4 show results for models K1–K12 (see the model parameters in Table 2). The upper panels show the gas temperature and the total H nucleus density profile; the middle panels show the density profiles of H$^0$, H$^+$, H$^-$, H$_2^0$ and H$_2^+$, and the bottom panels show the emissivity profiles of H$_2$ 1–0 S(1), H$^\alpha$, [N II] 6583, [O III] 5007 and [O I] 63 $\mu$m.

The gas temperature decreases with depth from the local diffuse gas value at the border of the CK to the 100-K limit assumed for...
our calculations. In the interface, the gas is hot, with temperatures $T > 2000$ K. As previously mentioned, the balance between the energy gain and loss by the gas determine its temperature. Fig. 5 shows the rate of energy gain and loss inside the CK model K4. The results are analogue for other models. In the interface, atomic processes dominate the heating and cooling of the gas, as in the diffuse ionized gas around the CK. The H$_2$ molecule dominates the heating and cooling in the core of the CK, while atomic mechanisms contribute to about 10 per cent of the total rates of energy loss and gain. Collisional excitation and de-excitation of H$_2$ are the most important mechanisms of loss and gain, respectively. Photoionization of H$_2$ may also contribute to the energy gain (<10 per cent). Heating by the photoelectric effect on grains may be significant only if $M_d/M_g \gg 10^{-2}$. For example, this mechanism contributes less than 1 per cent to the total energy input in model K4 ($M_d/M_g = 10^{-3}$) and less than 5 per cent for model K7 ($M_d/M_g = 10^{-2}$). The calculated grain temperature inside the CKs is approximately 20 K.

The transition between ionized and neutral H occurs in the interface, around $T \sim 8000$ K. Below this temperature and down to 100 K, hydrogen is mostly neutral. The density of molecular hydrogen increases inwards within the CK, reaching a fractional abundance in excess of 30 per cent. In cases with a high dust-to-gas ratio (see Section 3.2.1), a fully molecular region is produced while the temperature is still above 100 K. For other dust-to-gas ratios, the fully molecular region must have lower temperatures. The relative densities of H$^-$, H$_2^+$ and H$_3^+$ are smaller than $10^{-7}$ in all the models.

According to our models, inside a CK the most important H$_2$ formation mechanisms are:

(F1) $H + H^+ \rightarrow H_2 + e^-$,
(F2) $H^+_2 + H \rightarrow H^+ + H_2$,
(F3) $H^+_2 + e^- \rightarrow H_2 + H$,
(F4) $2H + \text{grain} \rightarrow H_2 + \text{grain}$,
and the main H$_2$ destruction mechanisms are:

(D1) $H_2 + h\nu \rightarrow H^+_2 + e^-$,
(D2) $H_2 + h\nu \rightarrow 2H$,
(D3) $H_2 + h\nu \rightarrow H^+_2 \rightarrow 2H$,
(D4) $H_2 + H^+ \rightarrow H + H^+_2$,
(D5) $H_2 + H^+_2 \rightarrow H_3^+ + H$,
(D6) $H_2 + H \rightarrow 3H$.

Both neutral and ionized species are involved in the H$_2$ formation and destruction processes; UV photons are important for the destruction of the molecule. Fig. 6 shows the rate of these processes as a function of the distance inside a CK. The associative detachment (F1) and the charge exchange (F2) reactions dominate the formation of H$_2$ at the border of the CK facing the star. The associative detachment is less important towards high depths, while the formation on grain surfaces becomes more important and dominates the H$_2$ formation in the CK core. The charge exchange and ion–molecule (F3) reactions contribute significantly to the molecular formation in the whole studied region.

The list of important reactions of H$_2$ formation and destruction in CKs is similar to the important reactions for the diffuse ionized...
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Figure 3. Same as Fig. 2 for models K5–K8 (left to right). Note the different density scale for model K8 in panel (a8).

As shown in Figs 2–4, models with different input parameters yield different ionization structures and hence result in different line emissivity profiles. Fig. 2 shows models with different CK density profiles (models K1–K4). Using the parameters of model K4 as reference, in models K5 and K6 we change the interface thickness, in model K7, the dust-to-gas ratio and in model K8, the core density (Fig. 3). Models K9–K12 have different distances from the central star (Fig. 4). Fig. 7 summarizes the effect of the input parameters on the total thickness from the border of the knot to the position where $T = 100$ K (i.e. $\Delta R_f$). The figure also shows the thickness of ionized and neutral zones of this region. Here the boundary between the ionized and neutral zones is assumed to be where H ionization degree is 0.5.

The thickness of the CK ionized zone increases significantly from type 1 to type 4 interface. The variation of the thickness of the neutral zone is less significant, but it also changes with the type of the interface. The model with type 1 interface has the smallest absolute thickness, while that with type 2 interface has the greatest value. As a result, $\Delta R_f$ increases significantly from type 1 to type 4 interface.

The density profile in the interface may result from the physical processes occurring and the nature of knots. For example, an $r^2$ function would be expected in the case of a spherical equilibrium outflow (Burkert & O’Dell 1998). According to Burkert & O’Dell (1998), the H$_\alpha$ surface brightness profile is better fitted by an exponential function than by an $r^2$ function (resulting from an $r^2$ increase in density). Following the results of Burkert & O’Dell (1998), we assume an exponential increase hereafter.

The thickness of the ionized zone and $\Delta R_f$ increase for models with thicker interfaces (greater $\Delta R$), as can be seen by comparing models K5, K4 and K6 (Figs 2 and 3). The three models have the same parameters, except for $\Delta R$, which takes, respectively, the values 0.01, 0.2 and 0.5. In models with $\Delta R = 0.01$, the neutral region is about 10 times larger than the ionized, while for $\Delta R = 0.2$ they are about the same size.

The rate of H$_2$ formation on grain surface is proportional to the dust-to-gas ratio. The contribution of dust to the gas energy input...
also increases in models with higher $M_d/M_g$, producing a more extended region with $100 < T < 300$ K. This allows hydrogen to become fully molecular in such a region. See, for example, models K4 and K7, in Figs 2 and 3. These models differ only by the value of dust-to-gas ratio. The dust-to-gas ratio for K7 is 10 times larger than for K4.

Density and gas temperature profiles for model K8 are shown in Fig. 3. This model is similar to model K4, but with a higher core density $n_K$. Comparing both models, it can be seen that both ionized and neutral regions reduce in size in the denser model. Several mechanisms can contribute to this difference, such as the increase in the radiation extinction by gas and dust, increase in the $\text{H}_2$ formation on grain surface and heating of the gas. It is important to note that, since we keep the dust-to-gas ratio constant throughout the model, an increase in the gas density implies an increase of the dust density.

An important parameter to the ionization structure of the CKs is the distance from the central star, since the ionizing flux and spectrum may change significantly with the position in the nebula. CKs farther from the central star have smaller ionized zones. If the CK is beyond the Helix ionization front, there is no ionized region, and the knot is completely neutral (see model K12 in Fig. 4).

### 3.3 Warm H$_2$ 1–0 S(1) emission

As can be seen in Figs 2–4 the emissivity of the H$_2$ 1–0 S(1) line in the CKs is high in a warm region, where the temperature ranges between 300 and 7000 K. The peak in the 1–0 S(1) emissivity in the studied region occurs where the density is around 40 per cent of the core density (with the exception of interface type 1 models, which have no intermediate density). This is also true for other rovibrational lines. This component of the H$_2$ emission can explain the excitation temperatures around 900–1800 K found by Cox et al. (1998) and Matsuura et al. (2007). The spatial width of the peak in the H$_2$ 1–0 S(1) emissivity is similar for all models, but the peak emissivity decreases with the distance from the central star.

Inside the CKs, the H$_2$ rovibrational levels of the ground electronic state are mainly excited and de-excited by collisional processes, particularly for lower $J$ levels. Formation pumping may contribute to high $J$ level population ($J > 10$), in the region where H is neutral. In such a region, rovibrational radiative de-excitation is an important mechanism for the population of levels with $J > 15$ or for lower $J$ levels with $v \sim 5$. UV Pumping is important for the population of levels with $v > 4$ and lower $J$.

Fig. 8 shows the H$_2$ excitation diagram for model K9. The effective column densities of the rovibrational levels $v = 0, 1, 2$ and 3 were calculated using the intensities determined in our model: these are indicated by the filled symbols. The lines in Fig. 8 represent Boltzmann distributions for three different temperatures. Different regions within the CK contribute to different parts of this plot. The highest energy levels are populated by collisions in the hottest regions of the CK. The lower energy levels are populated throughout the knot, at a range of temperatures. As a result, the integrated spectrum yields a much higher temperature for transitions involving a high upper energy level. The plot clearly shows these different excitation components of the H$_2$ emission. The lines of the band 1–0 and 2–1 are well represented by an excitation temperature of approximately 2000 K. The 0–0 band shows a distribution of lower

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**Figure 4.** Same as Fig. 2 for models K9–K12 (left to right).
temperatures, approximated in the plot as two components, with excitation temperatures of 900 and 200 K.

Effective column densities obtained from peak intensities measured by Matsuura et al. (2007) (their region a) are shown in Fig. 8 (open symbols). The agreement between the excitation temperatures of the model and the observations is evident. Matsuura et al. (2007) found a temperature of 1800 K from the 1–0 and 2–1 bands in a knot relatively close to the star, well represented by the model for these bands. (Note that the observed knot is 150 arcsec from the star, while the model is for a, deprojected, distance of 210 arcsec.)

For the 0–0 band, Cox et al. (1998) found from Infrared Space Observatory observations that the observed column densities obtained from lines S(2) to S(7) are well represented by Boltzmann distribution at a temperature around 900 K. This agrees with the excitation temperature of 1000 K predicted by the current model.

Matsuura et al. (2007) suggested that the different excitation temperatures they found (inferred from rovibrational lines) and the value obtained by Cox et al. (1998) (from pure rotational lines) are evidence for temperature variation within the nebula. Hora et al. (2006) found some indication for a gradient in the excitation in the Helix CKs with the distance from the central star, but in our models, a significant gradient is expected only at large distances, close to the ionization boundary of the PN. Instead, the different excitation temperatures found by Cox et al. (1998) and Matsuura et al. (2007) can be explained by the effect of the excitation within a single CK.

Using the ratios between lines of the S and Q branches of band 1–0 lines departing from the same level and assuming an extinction law.
of the form \( \lambda^{-1.7} \) (see Davis et al. 2003), we estimate an extinction of about 10–20 per cent at 2 \( \mu \)m. The model assumes that the knot is fully transparent, while in reality a fraction of the emission from the backside of the knot is extinct. However, this will not have a major effect on our results.

For comparison with \( H_2 \), the emissivity of a few intense atomic lines are also shown in Figs 2–4. The \([\text{Ne III}]\lambda 6583\) emission is produced in the interface of the CKs. \( H\alpha \) is also produced in the interface region, but there is a less intense extended emission region produced by the high-energy photons (which ionize the \( H \) atoms; the following recombination produces the line). The emissivity of the \([\text{Ne I}]\) line loses importance for models farther from the central star. For such models, the \([\text{Ne II}]\) line is produced only near the border of the CK, and its emissivity profile becomes very different from that of \( H\alpha \). Such behaviour may explain the separation between the \( H\alpha \) and \([\text{Ne II}] \) peaks observed by O’Dell et al. (2000). The decrease with distance of the \([\text{Ne II}] \) emissivity is stronger than for the 1–0 \( S(1) \) line, which can explain why all CKs with \([\text{Ne II}] \) emission have a 1–0 \( S(1) \) counterpart, while the opposite is not true, as observed by Matsuura et al. (2009).

Inside the CKs, the \([\text{O III}]\lambda 5007 \) emission is only produced in the interface and in models closer to the central star. In such cases, the emissivity inside the CK increases only up to one order of magnitude from the diffuse gas value, a small value when compared to other lines, such as \( H\alpha \) or \([\text{Ne II}] \) \( 6583 \). Images of the Helix show \([\text{O III}] \) emission in the diffuse gas and, in some cases, in the tip of CKs (O’Dell et al. 2007). According to Walsh & Meaburn (1993), 40 per cent of the CKs do not show any emission in \([\text{O III}] \) images.

The predicted emissivity of the IR fine structure line \([\text{O I}] \) 63 \( \mu \)m inside the CKs is very high as can be seen in Figs 2–4. Reay et al. (1988) found a correlation between the \( H_2 \) 1–0 \( S(1) \) and the optical \([\text{O I}]\lambda 6300 \) in a sample with several PNe, including the Helix. The optical line is produced only in the interface, while the profile of the IR \([\text{O I}] \) line is more similar to the one of 1–0 \( S(1) \).

As discussed before, if the CK is beyond the Helix ionization front, there is no ionized region, and the knot is completely neutral (see models K11 and K12 in Fig. 4). In this case, the emissivity of both \([\text{Ne II}]\) and \([\text{O I}] \) lines mentioned above is very low in the CKs and would not be detected.

### 3.4 \( H_2 \) 1–0 \( S(1) \) surface brightness

Measurements of the \( H_2 \) 1–0 \( S(1) \) line surface brightness of some representative CKs in the Helix nebula are plotted in Fig. 9. We identified 10 isolated CKs detected both in \( H\alpha \) and \( H_2 \) images. We measured 2.12-\( \mu \)m \( H_2 \) intensities from the images obtained by Matsuura et al. (2009). To calibrate the intensities, we used five stars within the observed field to measure the zero-point. We assume that the 2MASS \( K^* \) magnitude of these stars are the same as the magnitudes in \( H_2 \) filter. We apply a 25-pixel radius for aperture photometry and take the 35–50-pixel ring for the background measurements. The pixel scale is 0.117 arcsec. Table 3 lists the knot positions and the measurements.

Curves in Fig. 9 show the calculated \( H_2 \) 1–0 \( S(1) \) surface brightness of CK models as a function of the CK distance to the central star. The calculated surface brightness was averaged over the same aperture as the measurements to allow direct comparison. Different curves represent different \( \Delta R \) and CK radius. The surface brightness increases with a decrease of \( \Delta R \), an increase of the CK radius. CKs closer to the central star tend to have higher 1–0 \( S(1) \) surface brightness. The decrease in the \( H_2 \) 1–0 \( S(1) \) surface brightness with distance from the central star was also noted by O’Dell et al. (2007). If the CK is beyond the Helix ionization front, the 1–0 \( S(1) \) surface

![Figure 8](https://example.com/figure8.png)

**Figure 8.** \( H_2 \) excitation diagram. The effective column density was calculated from the surface brightness at the peak intensity of 1–0 \( S(1) \). Open symbols represent observations and filled symbols represent models. Lines are Boltzmann distributions for the temperature indicated near each curve.

![Figure 9](https://example.com/figure9.png)

**Figure 9.** \( H_2 \) 1–0 \( S(1) \) surface brightness of a CK as a function of the distance to the central star. Sets of solid, dashed and dot–dashed curves represent models with \( \Delta R = 0.5, 0.2 \) and 0.01 arcsec, respectively. Different curves within each set represents CK radius of 0.5, 1.0 and 2.0 arcsec, with the surface brightness increasing for larger CK radius. Dots represent measured values. The uncertainty in the distance is estimated assuming that the Helix symmetry axis is inclined 37° with respect to the line of sight.

| RA (E2000) | \( \delta \) (E2000) | Distance (arcsec) | Peak surface brightness (erg cm\(^{-2}\) s\(^{-1}\) sr\(^{-1}\)) |
|-----------|-----------------|------------------|----------------------|
| 22:29:45.987 | -20:49:05.98 | 125 | \( 2.0 \times 10^{-5} \) |
| 22:29:42.852 | -20:49:01.39 | 95 | \( 3.7 \times 10^{-5} \) |
| 22:29:42.873 | -20:47:43.35 | 162 | \( 1.7 \times 10^{-5} \) |
| 22:29:47.370 | -20:47:37.92 | 199 | \( 1.2 \times 10^{-5} \) |
| 22:29:46.616 | -20:47:52.70 | 144 | \( 9.6 \times 10^{-6} \) |
| 22:29:41.285 | -20:47:14.67 | 183 | \( 9.2 \times 10^{-6} \) |
| 22:29:37.829 | -20:48:01.66 | 132 | \( 2.8 \times 10^{-5} \) |
| 22:29:42.820 | -20:48:27.77 | 122 | \( 1.3 \times 10^{-5} \) |
| 22:29:39.823 | -20:47:53.55 | 141 | \( 1.9 \times 10^{-5} \) |
brightness drops dramatically, since there would be no enough radiation or temperature to excite significantly the upper vibrational levels of the molecule. Models can reproduce the magnitude of observed surface brightness and its decrease with distance to the central star.

The 1–0 S(1) peak brightness is slightly higher for models with higher dust-to-gas ratio. The increase caused by changing the dust-to-gas ratio from $10^{-3}$ to $10^{-2}$ is about 20 per cent. The 1–0 S(1) peak brightness also increases with increasing $n_K$. The difference between the models with $n_K = 10^5$ and $10^6$ cm$^{-3}$ is up to 40 per cent (20 per cent in the models farther from the central star).

Matsuura et al. (2009) show that, for the same number of CKs, the outer ring shows twice the surface brightness as the inner ring. According to them, such difference may be caused by the diffuse gas or by the difficulty in isolating CKs in the images. Since we do not expect a significant contribution from the diffuse gas and the surface brightness decreases with the distance to central star, the second explanation seems more likely.

4 CONCLUSION

As discussed in the Section 1, some features of the CKs’ emission indicate that they are significantly affected by the radiation field produced by the Helix central star. In this paper, we use the photoionization code AANGABA to assess the contribution that photoionization may have on the molecular hydrogen emission, supporting that photoionization plays a major role in such objects, which is in agreement with previous results from O’Dell et al. (2007) and Henney et al. (2007).

Our Helix nebula model with no CKs indicates that emission of H$_2$ from ionized diffuse gas is not significant, agreeing with the observations that the H$_2$ emission of the Helix is associated with the CKs (Meixner et al. 2005; Matsuura et al. 2009).

We study CK models with different sets of input parameters, chosen to cover the range of values inferred from Helix observations. The important mechanisms of gas heating and cooling, formation and destruction of H$_2$, excitation and de-excitation of H$_2$ were determined.

The emissivity of the H$_2$ 1–0 S(1) line in the CKs is important in a region with temperatures between 300 and 7000 K. Such a warm component of the H$_2$ emission may explain the excitation temperatures of around 900–1800 K found by Cox et al. (1998) and Matsuura et al. (2007). The contribution of this warm region to the emission of rovibrational lines is very important. For pure rotational lines of the $v = 0$ level, the contribution of the colder regions should be significant. The excitation diagrams obtained from our models seem to agree very well with the observations. Comparison with measurements indicates that models can reproduce the magnitude of observed surface brightness.

An important parameter to the ionization structure of the CKs is the distance from the central star, since the ionizing spectrum may change significantly with the position in the nebula. CKs farther from the central star have smaller ionized zones. If the CK is beyond the Helix ionization front, then there is no ionized region, the knot is completely neutral and there would be no enough radiation or temperature to excite significantly the upper vibrational levels of the molecule. The 1–0 S(1) intensity would be very low.

Our results also indicate that the separation between the H$_2$ and [N II] peaks observed by O’Dell et al. (2000) may be an effect of the distance of the knot from the star, since for knots farther from the central star the [N II] line is produced closer to the border of the CK than H$_2$.

The decrease of the [N II] emissivity with the distance of the CK to the central star is stronger than for the 1–0 S(1) line, which can explain why all CKs with [N II] emission have a 1–0 S(1) counterpart, but the opposite is not true, as observed by Matsuura et al. (2009).

As pointed out by Burkert & O’Dell (1998), the interface between the diffuse gas and the CK core may provide important clues about the mechanisms that shape and sustain the PN CKs. Our models show that there are significant differences in the models’ results depending on the assumed density profiles of this region. Images that could resolve this region in great detail are then essential.

We find that the temperature derived from H$_2$ observations even of a single knot will depend very strongly on the observed transitions, with much higher temperatures derived from excited levels. This is caused by the large range of temperatures present, and the presence of significant amounts of molecular hydrogen within the mini-PDR. This explains the puzzling temperature differences found by previous observers.

We also find that H$_2$ required to fit the observations is consistent with the abundances calculated through equilibrium chemistry, with a variety of formation and dissociation reactions. There is no need to presume that the molecular hydrogen in the knots predate the ionization of the nebula, assuming that there is enough time to reach equilibrium. This does not resolve the issue of when and how the knots formed, but we cannot exclude models where the knots formed after the onset of ionization, nor models where the knots already formed in the AGB wind.

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REFERENCES

Aleman I., Gruenwald R., 2004, ApJ, 607, 865
Aleman I., Gruenwald R., 2011, A&A, 528, A74
Beckwith S., Gatley I., Persson S. E., 1978, ApJ, 219, L33
Benedict G. F. et al., 2009, AJ, 138, 1969
Bordas C., Cosby P. C., Helm H., 1990, J. Chem. Phys., 93, 6303
Burkert A., O’Dell C. R., 1998, ApJ, 503, 792
Cox P. et al., 1998, ApJ, 495, L23
Davis C. J., Smith M. D., Stern L., Kerr T. H., Chiar J. E., 2003, MNRAS, 344, 262
Gruenwald R. B., Viegas S. M., 1992, ApJS, 78, 153
Gussie G., Pritchet C., 1988, J. R. Astron. Soc. Canada, 82, 69
Harris H. C. et al., 2007, AJ, 133, 631
Henney W. J., Williams R. J. R., Ferland G. J., Shaw G., O’Dell C. R., 2007, ApJ, 671, L137
Henry R. B. C., Kwitter K. B., Dufour R. J., 1999, ApJ, 517, 782
Hora J. L., Latter W. B., Deutsch L. K., 1999, ApJS, 124, 196
Hora J. L., Latter W. B., Smith H. A., Marengo M., 2006, ApJ, 652, 426
Huggins P. J., Frank A., 2006, in Barlow M. J., Méndez R. H., eds, Proc. IAU Symp. 234, Planetary Nebulae in Our Galaxy and Beyond. p. 271
Huggins P. J., Bachiller R., Cox P., Forveille T., 1992, ApJ, 401, L43
Huggins P. J., Forveille T., Bachiller R., Cox P., Ageorges N., Walsh J. R., 2002, ApJ, 573, L55

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Kastner J. H., Weintraub D. A., Gatley I., Merrill K. M., Probst R. G., 1996, ApJ, 462, 777
Kwok S., 2000, The Origin and Evolution of Planetary Nebulae. Cambridge Univ. Press, Cambridge
Likkel L., Dinerstein H. L., Lester D. F., Kindt A., Bartig K., 2006, AJ, 131, 1515
Matsuura M. et al., 2007, MNRAS, 382, 1447
Matsuura M. et al., 2008, Messenger, 132, 37
Matsuura M. et al., 2009, ApJ, 700, 1067
Meaburn J., Clayton C. A., Bryce M., Walsh J. R., Holloway A. J., Steffen W., 1998, MNRAS, 294, 201
Meixner M., McCullough P., Hartman J., Son M., Speck A., 2005, AJ, 130, 1784
O’Dell C. R., Handron K. D., 1996, AJ, 111, 1630
O’Dell C. R., Henney W. J., Burkert A., 2000, AJ, 119, 2910
O’Dell C. R., Balick B., Hajian A. R., Henney W. J., Burkert A., 2002, AJ, 123, 3329
O’Dell C. R., McCullough P. R., Meixner M., 2004, AJ, 128, 2339
O’Dell C. R., Henney W. J., Ferland G. J., 2005, AJ, 130, 172
O’Dell C. R., Henney W. J., Ferland G. J., 2007, AJ, 133, 2343
Osterbrock D. E., Ferland G. J., 2006, in Osterbrock D. E., Ferland G. J., eds. Astrophysics of Gaseous Nebulae and Active Galactic Nuclei, 2nd. edn. University Science Books, Sausalito, CA
Péquignot D. et al., 2001, in Ferland G., Savin D. W., eds, ASP Conf. Ser.

Vol. 247, Spectroscopic Challenges of Photoionized Plasmas. Astron. Soc. Pac., San Francisco, p. 533
Reay N. K., Walton N. A., Atherton P. D., 1988, MNRAS, 232, 615
Schild H., 1995, A&A, 297, 246
Spaans M., Meijerink R., 2005, Ap&SS, 295, 239
Speck A. K., Meixner M., Fong D., McCullough P. R., Moser D. E., Ueta T., 2002, AJ, 123, 346
Speck A. K., Meixner M., Jacoby G. H., Knezek P. M., 2003, PASP, 115, 170
Stasińska G., 2009, preprint (arXiv:0704.0348)
Stasińska G., Szczerba R., 1999, A&A, 352, 297
Stasińska G., Tylenda R., 1986, A&A, 155, 137
Sterling N. C., Dinerstein H. L., 2008, ApJS, 174, 158
Tarter C. B., Salpeter E. E., 1969, ApJ, 156, 953
Tenenbaum E. D., Milam S. N., Woolf N. J., Ziurys L. M., 2009, ApJ, 704, L108
Tielens A. G. G. M., 1993, in Weinberger R., Acker A., eds, Proc. IAU Symp. 155, Planetary Nebulae. Kluwer, Dordrecht, p. 155
Tielens A. G. G. M., Hollenbach D., 1985, ApJ, 291, 722
Volk K., Hrivnak B. J., Kwok S., 2004, ApJ, 616, 1181
Walsh J. R., Meaburn J., 1993, Messenger, 73, 35

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