Near-infrared spectroscopy of (proto)-planetary nebulae: molecular hydrogen excitation as an evolutionary tracer

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ABSTRACT
We present an in-depth analysis of molecular excitation in 11 H2-bright planetary and protoplanetary nebulae (PN and PPN). From newly acquired K-band observations, we extract a number of spectra at positions across each source. H2 line intensities are plotted on ‘column density ratio’ diagrams so that we may examine the excitation in and across each region. To achieve this, we combine the shock models of Smith, Khanzadyan & Davis with the photodissociation region (PDR) models of Black & van Dishoeck to yield a shock-plus-fluorescence fit to each data set.

Although the combined shock + fluorescence model is needed to explain the low- and high-energy H2 lines in most of the sources observed (fluorescence accounts for much of the emission from the higher-energy H2 lines), the relative importance of shocks over fluorescence does seem to change with evolutionary status. We find that shock excitation may well be the dominant excitation mechanism in the least evolved PPN (CRL 2688 – in both the bipolar lobes and in the equatorial plane) and in the most evolved PN considered (NGC 7048). Fluorescence, on the other hand, becomes more important at intermediate evolutionary stages (i.e. in ‘young’ PN), particularly in the inner core regions and along the inner edges of the expanding post-asymptotic giant branch (AGB) envelope. Since H2 line emission seems to be produced in almost all stages of post-AGB evolution, H2 excitation may prove to be a useful probe of the evolutionary status of PPN and PN alike. Moreover, shocks may play an important role in the molecular gas excitation in (P)PN, in addition to the low- and/or high-density fluorescence usually attributed to the excitation in these sources.

Key words: circumstellar matter – ISM: jets and outflows – ISM: kinematics and dynamics – ISM: lines and bands – infrared: stars.

1 INTRODUCTION
The evolution of stars from the asymptotic giant branch (AGB) to the planetary nebula (PN) phase involves a short-lived transition through the so-called protoplanetary nebula (PPN) phase (Kwok 1993). The central stars of PPN are still too cool to ionize the shell of detached, slow-moving circumstellar material ejected during the AGB phase, yet they do drive high-velocity winds (powered by radiation pressure), which impinge on and shape the AGB shell. A decreasing equatorial-to-polar density gradient in the AGB envelope probably causes the bipolar nebula morphologies evident in optical and near-infrared (near-IR) images of both PPN and PN (the fact that PPN are asymmetric suggests that this process starts early, within a few hundred years of the AGB phase). As the central source of the PN (the CSPN) evolves and its temperature increases the inner cavity becomes ionized. This cavity will likewise propagate more rapidly along the polar axis, magnifying the original density contrast. These dynamical processes, when combined with the effects of differing orientation with respect to the observer, probably explain many of the apparent morphological classes of PN, the most common being ‘face-on’ ring and elliptical, or ‘edge-on’ bipolar structures (e.g. Balick 1987).

Infrared observations are potentially very useful for probing the interaction between the fast atomic/ionized winds and the dense, molecular AGB envelopes associated with evolved stars. The near-IR bands include emission lines from highly excited atoms and
ions as well as rovibrationally excited molecules such as CO and H$_2$. Near-IR studies are also less hampered by extinction than similar optical studies, and yet data with high spatial and spectral resolution can still be obtained. H$_2$ observations, in particular, may be used to trace the excited molecular environment in PN and PPN; they may be used to distinguish between gas excitation mechanisms, to quantify the relative importance of thermal and non-thermal excitation processes, and as a probe of the shock physics. For example, the recent spectroscopic survey of Hora, Latter & Deutsch (1999) points to a combination of thermal and non-thermal (fluorescent) excitation in PN, while in a few PPN, new, high-resolution images reveal what appear to be molecular ‘bow shocks’ along the poles of the nebulae (Cox et al. 1997; Sahai et al. 1998a), which suggests that shock excitation may also play a role.

In this paper we present low-resolution $K$-band spectroscopy of a range of PPN and PN. Background details on the individual targets are given in Tables 1 and 2. Our data complement the recent surveys of Hora et al. (1999) and Lumsden, Puxley & Hoare (2001). Only three of our sources are found in these earlier surveys. Our source sample, though more limited, includes targets over a wide range of evolutionary and morphological stages; e.g. bipolar PPN (AFGL 2688, M 1-92, IRAS 17150−3224 and 17441−2411), compact, optically bright PPN (IRAS 22272+5435), ‘young’ PN (IRAS 21282+5050) and more evolved PN systems (NGC 7048, NGC 6445, Hb 5), as well as two of the highest-excitation PN known (NGC 6302 and 6445) and the rapidly evolving post-AGB/young-PN IRAS 18062+2410. Although all of our PN targets were known to be bright in H$_2$ 2.122-µm emission (from published imaging surveys; e.g. Kastner et al. 1996; Cox et al. 1997), we have also obtained new images of the PN sample, to illustrate the distribution of H$_2$ emission at (in some cases) better spatial resolution and to more accurately measure the surface brightness in each source. In contrast, near-IR observations of only a few of the PN (CRL 2688, M1-92, IRAS 17150−3224 and 17441−2411) have previously been published (Bujarrabal et al. 1998a; Sahai et al. 1998b; Weintraub et al. 1998; Hora et al. 1999; García-Hernández et al. 2002).

From observations and modelling of the neutral gas in planetary nebulae (e.g. Dinerstein et al. 1988; Graham et al. 1993; Hora & Latter 1994; Natta & Hollenbach 1998; Shupe et al. 1998; Hora et al. 1999; Vicini et al. 1999; Lumsden et al. 2001) the vibrationally excited H$_2$ lines at $\sim$2 µm are often thought to be produced in a dense PDR, where thermal emission derives from warm ($\sim$1000 K), dense gas that is heated by grain photoelectric heating and by far ultraviolet (FUV) pumping of H$_2$. As the source ages and expands, however, the molecular gas density drops and only then can the lower-energy H$_2$ states be populated by non-thermal excitation (fluorescence), and then only for low-mass central stars. However, shocked H$_2$ emission from the boundary between the fast wind and dense AGB envelope may also contribute to the emission spectrum, and even dominate over the PDR emission if the mass-loss rate is high ($>10^{-5}$ M$_\odot$ yr$^{-1}$; Natta & Hollenbach 1998). Notably, H$_2$ emission is not observed in all PN. It is usually only detected in bipolar nebulae (Kastner et al. 1996; Weintraub et al. 1998; García-Hernández et al. 2002). These in turn have been associated predominantly with a high mass-loss rate and a high-mass progenitor (e.g. Corradi & Schwartz 1995). Moreover, as we note in our description of each source in Section 3, high wind velocities – and presumably high shock velocities – are inherent to each target. To interpret the data from our sample of H$_2$-bright sources, it therefore seems prudent to consider a model that incorporates shock and fluorescent excitation.

We therefore apply fluorescent/PDR models published in the literature (Black & van Dishoeck 1987) combined with shock theory that we have developed to analyse the spectra of Herbig–Haro objects (e.g. Smith, Brand & Moorehouse 1991a,b; Smith 1995; Davis et al. 1999; Smith et al. 2003). After briefly considering individual line ratios, we adopt the column density ratio (CDR) method (e.g. Burton & Haas 1997). This is potentially a very powerful tool, since one may extract the mean extinction, relative fluorescent and shock contributions to the gas excitation and the H$_2$ ortho–para ratio for the fluoresced gas. We also search for a correlation between H$_2$ excitation and the evolutionary state of each target, and look for changes in excitation spatially across each target (in the case of CRL 2688 along the polar and equatorial axes).

### 2 OBSERVATIONS AND DATA REDUCTION

Low-resolution ($R \sim 400$) $K$-band spectra were obtained at the UK Infrared Telescope (UKIRT) using the facility Cooled Grating Spectrometer CGS 4 (Mountain et al. 1990) on 1999 July 17–19 and 2000 June 30 (Table 1). With the 40 line mm$^{-1}$ grating and the 300 mm focal length camera the pixel scale measures 0.61 arcsec; a 2-pixel wide slit was employed throughout. For all sources, object–sky–sky–object sequences were repeated to facilitate sky-subtraction and build up signal-to-noise ratio, the telescope being nodded an arcmin or so off-source for many of the targets. For the more compact objects the source was nodded up and down the slit, thereby doubling the on-source integration time. At each ‘object’ or ‘sky’ position four 30-s exposures were obtained, the array being stepped in half a spectral resolution element per exposure to fully sample the instrumental resolution and correct for bad pixels.

Point and compact sources were ‘peaked-up’ so that their bright, central continuum were on the same central reference row on the array. For extended sources, a nearby reference (CMC) star was peaked-up on the same spectrometer row (to correct the absolute pointing), and the telescope then slewed to the target coordinate listed in Table 1. Slit position angles were set so that the slit ran along the extended (bipolar) axis of each target, if known; in the case of CRL 2688, two orthogonal slit positions were observed (see Table 1 and Fig. 1a).

<table>
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<th>Table 1. Observing log.</th>
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<td><strong>Target</strong></td>
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<td>NGC 6302</td>
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<td>IRAS 17150−3224</td>
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<td>IRAS 17441−2411</td>
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<td>Hb 5</td>
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<td>NGC 6445</td>
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<td>NGC 6886</td>
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<td>CRL 2688 (disc)</td>
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<td>CRL 2688 (jet)</td>
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<td>NGC 7048</td>
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<td>IRAS 21282+5050</td>
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<td>IRAS 22272+5435</td>
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<sup>1</sup>Position of slit on each target (this is not necessarily the geometrical centre of the PN or PPN, although for the more compact, point-like sources the slit was centred on the continuum peak – see Fig. 1 for slit positions).

<sup>2</sup>UT date observed (year/month/day).

<sup>3</sup>Position angle, measured east of north.
Each spectral image was bias-subtracted, flat-fielded (using observations of an internal blackbody source), corrected for optical distortions (so that sky or arc lines ran down columns) and then wavelength calibrated using argon arc spectra and routines available in the STARLINK package FIGARO. For extended sources, groups of rows were extracted and co-added at a few locations along each slit; the number of adjacent, 0.6-arcsec wide rows used, and the locations of these rows along the slit were arbitrarily chosen for each target, the aim being to maximize the signal-to-noise ratio in each co-added spectrum, though also to give data at a few positions across each target (if possible). The areas used for each source are illustrated in Fig. 1; the ‘up’ and ‘dn’ labels refer to relative positions in each spectral image, rather than specific positions on the sky. For sources that were nodded along the slit (the compact targets), both positive and negative beams were extracted and co-added. All spectra were subsequently de-rippled and corrected for telluric absorption effects using an F- or A-type subgiant or dwarf standard star spectrum, if present in the standard star spectrum, were removed.

From Skinner et al. (1997).

H2 line emission detected toward IRAS 17441−2411 by Weintraub et al. (1998).

The morphologies of these targets are confirmed with published HST imaging.
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Figure 1. Narrow-band 2.122-μm images of two of the PPN (CRL 2688 and M 1-92) and six of the PN. The dashed lines indicate the position and angles of the slits used in each case; the areas along each slit over which spectra were extracted and added are also indicated with white blocks.

object and standard-star spectra become increasingly noisy due to the drop-off in atmospheric transmission and blocking-filter efficiency. Telluric absorption features are not always properly removed in these regions, and line strengths measured in these regions are less certain.

Finally, the FIGARO routine GAUSS was used to fit continua and measure line intensities in each reduced spectrum. Where lines were blended (notably the Q-branch lines at 2.40–2.45 μm and occasionally the H₂ and H lines near 1.95 μm) the routine FITGAUSS was used to fit multiple Gaussian components to the blend (a constant continuum level across the region fitted is assumed; since this usually was not the case, GAUSS was used to fit the curving continuum across the spectrum; the fit was then subtracted from the spectrum before the multicomponent Gaussian fitting with FITGAUSS was attempted).

Narrow-band images of eight of the more extended sources were also obtained via the Service Observing programme at UKIRT. The data were obtained with the common-user 1–2.5 μm imager UFTI on 2000 July 9, 2001 May 20 and September 12. UFTI employs a 1024 × 1024 HgCdTe Hawaii array, and has a plate scale of 0.091 arcsec pixel⁻¹, giving a field of view of 92 arcsec. Five-point mosaics were obtained of each target, through 2.122 μm (Δλ = 0.02 μm) H₂ 1–0 S(1) and 2.270 μm (Δλ = 0.02 μm) K-band continuum filters; an exposure time of 100 s was adopted throughout. Individual frames were bad-pixel-masked, dark-subtracted and flat-fielded (using separate sky flat-field frames obtained just prior to the PN data) before registration and mosaicking. The ORAC pipeline software was used to reduce the data in this way. UKIRT faint standard stars (Hawarden et al. 2001) were also obtained for flux-calibration (except for the image of CRL 2688, Fig. 1a, which is not calibrated).

3 RESULTS

The sources observed are listed in Tables 1 and 2. Our goal was to observe a representative sample of post-AGB, PPN and PN, and at the same time obtain sufficiently deep spectra so that we could measure line intensities at a number of locations across each source. K-band spectra of some of our targets were recently presented as part of an extensive (JHK) survey by Hora et al. (1999). Prior to this, Hrivnak, Kwok & Geballe (1994) had obtained H-, K- and L-band spectra of a number of PPN; again, a few of these sources were observed in this study (see below). Many of our PN targets have also been imaged previously in the near-IR (e.g. Latter et al. 1995; Kastner et al. 1996; Sahai et al. 1998b), though some of the PPN (listed as IRAS sources here) are newly discovered compact, bipolar nebulae for which no near-IR data have been published.

Below we discuss each target individually. In Figs 1 and 2 we show narrow-band images of eight of the more extended sources.
These show the positions of the slits observed, and the locations and spatial extents of the extracted spectra. The contour plots in Fig. 2 also give some indication of the H$_2$ 1–0 S(1) surface brightness across each source. The extracted spectra are shown in Figs 3–13 in the following sections. From each spectrum we have measured line intensities; we plot these on column density ratio diagrams in Figs 14–18. The CDR technique is described further in Section 4.

3.1 Protoplanetary nebulae (and young PN)

3.1.1 CRL 2688

CRL 2688 (AFGL 2688; the ‘Egg’ nebula) is a well-known, bright, bipolar PPN (e.g. Ney et al. 1975; Cox et al. 1997; Skinner et al. 1997; Sahai et al. 1998a,b). CRL 2688 is very much the archetypal PPN: the progenitor star, a carbon-rich supergiant, is thought to have left the AGB approximately 200 yr ago and is now on the horizontal track of the Hertzsprung–Russell (HR) diagram. Its spectral energy distribution (SED) exhibits excess flux in the far-IR (associated with the warm AGB envelope), while the presence of atomic fine-structure lines in ISO spectra are consistent with a cool central star that has not yet photodissociated the molecular AGB envelope (Cox et al. 1997; Skinner et al. 1997).

In the optical CRL 2688 is clearly bipolar. However, early near-IR images of CRL 2688 revealed H$_2$ emission regions in both the north–south bipolar lobes and in an east–west equatorial plane (Latter et al. 1993). Spectroscopic studies show that the northern and eastern regions are blueshifted, while the southern and western are redshifted. These data have since been interpreted in terms of shock excitation along a bipolar jet and in an equatorial AGB wind/torus by a poorly collimated, fast, post-AGB wind. In addition to these features, more recent high-resolution (optical) Hubble Space Telescope (HST) images reveal a pair of ‘searchlight beams’ associated with each bipolar lobe, which emerge from a dark, equatorial lane that obscures the central source. Superimposed on to these beams are a series of arcs with centres of curvature situated close to the central star (Sahai et al. 1998a,b). Sahai et al. interpret these pairs of beams in terms of annular holes coaxial with the polar axis, that were carved out by a high-velocity flow. The arcs may then be associated with periods of increased outflow activity during the AGB mass-loss phase.

In the infrared, HST NICMOS images in H$_2$ show the northern and southern H$_2$ features to be elongated ‘bubbles’ that are capped with bright, bow-shock-like emission knots. These bubbles align precisely along the polar axes of the nebula (PA $\sim$ 19°) and lie between the two optical, search-light beams described above (Sahai...
Figure 2. Contour plots showing the continuum-subtracted 2.12-µm images of the target (P)PN. The contours in each plot start at $1.5 \times 10^{-18} \text{W m}^{-2} \text{arcsec}^{-2}$ and increase in linear intervals of $1.5 \times 10^{-18} \text{W m}^{-2} \text{arcsec}^{-2}$ except for NGC 7048 where the contours start at $1.0 \times 10^{-18} \text{W m}^{-2} \text{arcsec}^{-2}$ (interval = $1.5 \times 10^{-18} \text{W m}^{-2} \text{arcsec}^{-2}$), M 1-92 where the contours start at $1.5 \times 10^{-18} \text{W m}^{-2} \text{arcsec}^{-2}$ (interval = $3.9 \times 10^{-18} \text{W m}^{-2} \text{arcsec}^{-2}$), and CRL 2688 where the data are not flux calibrated (though the contours are still spaced linearly). Offsets are in arcsec from the nominal source position given in Table 1. North is up and East is left in all cases.

et al. 1998b). The near-IR bubbles and H$_2$ bow shocks probably represent the limb-brightened edges of a fast (few hundred km s$^{-1}$), collimated bipolar outflow that is impinging on and sweeping up the slower, dense, AGB wind. The equatorial H$_2$ features are resolved into individual arcs by HST. These features are difficult to explain, though their narrow, limb-brightened, arcuate morphologies point to a similar, shock-excitation mechanism. Based on H$_2$ and CO kinematics, Cox et al. (2000) suggest a model involving a fan of multipolar jets radiating outward from the central star, while Kastner et al. (2001) favour a model that combines radial expansion and
rotation about the polar axis; in both cases the equatorial H$_2$ emission is assumed to be shock-excited by a fast wind in the equatorial direction. The polar lobes and bow-shocks and the equatorial arcs can be seen in our ground-based images in Figs 1(a) and 2, though for a more spectacular representation see fig. 1 of Sahai et al. (1998b).

Near-IR spectra of CRL 2688 were first obtained by Thronson (1982) and more recently by Hora & Latter (1994) and Cox et al. (1997). Excitation analysis generally supports claims that shock-excitation (rather than fluorescence) is the dominant mechanism in both the equatorial and bipolar ‘jet’ lobes. We have obtained K-band spectra along two orthogonal slit positions, which include the polar and equatorial H$_2$ regions (Fig. 1a). Spectra were extracted at two locations in the N–S bipolar lobes, and at four positions along the E–W disc axis. We present these spectra in Fig. 3. H$_2$ emission lines are detected at all locations. Br is not detected in CRL 2688, as one would expect for a shocked, molecular environment where photoionization has not yet set in.

3.1.2 M 1-92

M 1-92 is a bipolar, oxygen-rich PPN, much like CRL 2688 and the IRAS sources discussed below. The temperature of its central star is quite high (~20 000 K), so M 1-92 is probably slightly more evolved than CRL 2688, and it could be approaching the transition phase from PPN to photoionized PN. Bujarrabal et al. (1998b) estimate a kinematic age of approximately 900 yr.

In optical images the nebula comprises two bipolar lobes of scattered polarized light (Herbig 1975; Trammell & Goodrich 1996; Bujarrabal et al. 1998a,b). Spectra from these lobes comprise a stellar continuum, plus scattered permitted Balmer and He I lines, and a variety of low-excitation forbidden emission lines that are inherent to the lobes. The latter are produced in Herbig–Haro-like bow shocks with velocities approaching 200–300 km s$^{-1}$ (Solf 1994). The NW lobe is optically brighter than the SW lobe, being inclined toward the observer at an angle of approximately 55° to the plane of the sky. The two lobes are separated by a lane of obscuration, although the central star is just visible because of the inclination of the system. In optical HST images the continuum in the lobes appears smooth, with no sign of arcuate structures such as those seen in CRL 2688, while the shock-excited [S II] and [O I] is shown to delineate a knotty, collimated jet that is roughly, though not precisely, aligned with the axis of the nebula (Trammell & Goodrich 1996; Bujarrabal et al. 1998a). Indeed, the jet may be precessing or ‘wiggling’ within the lobes of the nebula (Trammell & Goodrich 1996).

High-resolution CO maps reveal two hollow shells that envelope the bipolar lobes (Bujarrabal et al. 1998b). These dense, molecular shells likely contain the ejecta from the AGB phase; they contain most of the nebula material and are expanding at high speed (up to 70 km s$^{-1}$). The shells may represent gas swept up by the fast, post-AGB wind. Bujarrabal et al. also report the detection of fast molecular clumps or bullets at the tips of the bipolar lobes/shells (i.e. along the jet axes), and a dense, though expanding, equatorial torus, with a diameter of approximately 2–3 arcsec.

In Fig. 1(b) we present our narrow-band image of M 1-92. At 2 µm a single, ovoidal peak is observed, orientated with its long axis along the same axis as the bipolar lobes. The peak is centred on the central star; the lobes themselves are not resolved. Bujarrabal et al. (1998a) present a similar ground-based, near-IR image of M 1-92. They observe two knots of H$_2$ emission, one in each lobe; our continuum-subtracted image in Fig. 2 shows the same H$_2$ features along the polar jet axis. The H$_2$ knot in the NW lobe is triangular in appearance and is probably a bow shock, being more extended laterally than the optical knots observed along the jet axis (Bujarrabal et al. 1998a).

Hora et al. (1999) obtained JHK spectra toward the core and NW lobe of M 1-92; the latter corresponds to the ‘dn’ position in our data (see Figs 1b and 4). In this NW lobe, Hora et al. detect Br and the CO bandheads in emission. With our new spectra we can confirm their presence in both bipolar lobes. We also detect H$_2$ emission from both lobes (Hora et al. report a tentative detection in the NW lobe) though we do not detect H$_2$ toward the core region. The H$_2$/Br ratio is much lower in M 1-92 than it is in CRL 2688, consistent with the fact that M 1-92 is more evolved and associated with an ionized nebula.

3.1.3 IRAS 17150–3224 and 17441–2411

Recent optical HST images of IRAS 17150–3224 (AFGL 6815) and 17441–2411 illustrate their compact though bipolar morphologies (Kwok, Su & Hrivnak 1998; Su et al. 1998); indeed, both are morphologically similar to M 1-92 and CRL 2688. Both nebulae
Figure 4. H$_2$ was observed in the two lobes of the PPN M 1-92; no bright H$_2$ was detected toward the central region (although Br$\gamma$ and CO bandheads were detected in all three regions). The spectra presented are from the two bipolar lobes; the regions are labelled up (top spectrum) and dn (bottom spectrum) in Fig. 1(b). The first four CO bandheads are marked with arrows; Br$\gamma$ is marked with a cross; H$_2$ v = 1–0 transitions are marked with ticks.

are probably orientated close to the plane of the sky (i.e. with their equatorial tori viewed edge-on), so that their central stars are largely obscured at optical wavelengths. In the HST data, both sources also exhibit a series of concentric arcs superimposed on to their bipolar lobes (like CRL 2688), which again may be associated with spherically symmetric AGB mass loss (Kwok et al. 1998; Su et al. 1998). The SEDs of both objects clearly illustrate their PPN nature, being double-peaked though dominated by a strong IR component produced by their AGB envelopes (Kwok et al. 1996; Ueta, Meixner & Bobrowski 2000).

In the more extended of the two targets, IRAS 17150$-$3224, we obtained spectra at three positions (Fig. 5). The spectra are associated with the SW lobe (top spectrum), the bright core and the NE lobe (bottom). We did not obtain a near-IR image of this nebula, though the bipolar lobes are clearly seen in the optical HST images (Kwok et al. 1998). Strong H$_2$ emission is detected in both bipolar lobes; indeed H$_2$ seems to be brightest in these lobes, as one might expect of emission associated with the interaction of a fast wind with the AGB shell. In comparison, weak Br$\gamma$ emission is detected predominantly toward the core region.

Our spectrum of IRAS 17441$-$3224, which is of fairly low signal-to-noise ratio, does not show H$_2$ emission in either the core or the lobes (so it is not presented here). We also do not see CO bandheads, though Br$\gamma$ is seen in absorption.

Weintraub et al. (1998) report the detection of H$_2$ emission towards the core regions in both nebulae. They postulate that this emission may be associated with an expanding equatorial torus, similar to that seen in H$_2$ in CRL 2688. Their spectra were obtained with an east–west slit and at high spectral resolution. The orientation of their slit (not aligned with the bipolar lobes of either nebula) may explain why they did not detect extended emission in the lobes of either source, particularly IRAS 17150$-$3224 where we do detect bright H$_2$ line emission. Their higher spectral resolution might also then explain why they were able to detect line emission in the central region in IRAS 17441$-$3241 against the strong continuum from the CSPN, when we were not (the orientation of our CGS4 slit along the bipolar lobes would of course also hinder our detection of extended, equatorial emission). Weintraub et al. did find that the H$_2$ in IRAS 17441$-$3241 was much fainter than in IRAS 17150$-$3224.

3.1.4 IRAS 18062+2410

IRAS 18062+2410 (= V886 Her) is an IRAS source with far-infrared colours similar to planetary nebulae (Volk & Kwok 1989). Optical spectra identify it as an early B-type post-AGB supergiant; its spectrum has absorption lines and the permitted and forbidden emission lines typical of young, high-density, low-excitation PN (Arkhipova et al. 1999; Parthasarathy et al. 2000). Significantly, IRAS 18062+2410 seems to be evolving very rapidly, from post-AGB to the PN phase; in the last 50 yr it has evolved from an A5 star to a Be star. It has only recently become hot enough to photoionize the ejected AGB envelope (massive post-AGB stars are thought to evolve from F0 to B1 in only ~100 yr; Blöcker 1995). IRAS 18062+2410 is therefore probably now in the early stages of the
PN phase. Parthasarathy et al. (2000) derive an effective temperature of 20,000 K for this object.

We present just one spectrum for this compact, point-like source (Fig. 6). The continuum in our \(K\)-band spectrum shows a decrease with wavelength (unlike the other compact, IRAS sources in our sample), as expected for the photosphere of a hot, though still slightly reddened object (Hrivnak et al. 1994). Nevertheless, we still detect strong \(H_2\) line emission, and equally bright \(Br\) recombination-line emission (in rough agreement with the similar observations of García-Hernández et al. 2002).

3.1.5 IRAS 21282+5050

Kwok, Hrivnak & Langill (1993) present a detailed optical and infrared study of this carbon-rich source. Their photometry and double-peaked SED plot suggest that the source might be a PPN, although it does exhibit weak radio continuum emission at 2 and 6 cm (Likkel et al. 1994), so we refer to this object as a ‘young’ PN, i.e. a nebula, such as IRAS 18062+2410, that is just beginning to be ionized (Meixner et al. 1997). In the optical IRAS 21282+5050 is marginally elongated N–S, and is possibly associated with an orthogonal molecular torus seen edge-on (Shibata et al. 1989; Kwok et al. 1993; Meixner et al. 1997). IRAS 21282+5050 is also associated with a WC11 central star (Menzies & Wolstencroft 1990).

IRAS 21282+5050 is included in the survey of Hora et al. (1999), who obtain near-IR spectra at two positions, toward the core and toward a position offset 3 arcsec N, 3 arcsec W. They detect \(H_2\) emission lines from the latter, and \(H\) i from the core position (similar to our observations of IRAS 17150−3224 described above). We present only one spectrum (the sum of six 0.61-arcsec wide rows across the nebula; Fig. 7). We find \(H_2\) 1–0 S(1) and \(Br\) emission lines of roughly equal strength when integrated over this region, again as one would expect for a young PN rather than a PPN.

3.1.6 IRAS 20000+3239 and 22272+5435

IRAS 20000+3239 and 22272+5435 were first identified as PPN by virtue of their IRAS colours and dust temperatures (Kwok, Hrivnak & Geballe 1995; Ueta et al. 2000). Both targets are more compact than some of the other IRAS objects discussed above (e.g. IRAS 17150−3224 and 17441−2411), so although we identify them as being ‘round’ or ‘elliptical’ in morphology (Table 2), future high-resolution imaging may show them to be bipolar in shape.

IRAS 22272+5435 is associated with an optically bright central star (Ueta et al. 2000). In fact, this is one of the brightest objects in our survey (Table 2). In comparison, IRAS 20000+3239 is a relatively faint source. This difference could be due to orientation and consequently, in the latter, obscuration of the central star by an equatorial torus or disc (as is the case for IRAS 17441−2411 and 17150−3224 discussed above). Of course, IRAS 20000+3239 could also be further away.

Hrivnak et al. (1994) present \(K\)-band spectra of IRAS 20000+3239 and 22272+5435. These data clearly exhibit both \(Br\) and \(CO\) bandheads (longward of 2.25 \(\mu\)m) in absorption. Remarkably, the \(CO\) bandhead in IRAS 22272+5435 was found to switch from absorption to emission over a 3-month interval. Hrivnak et al. suggest that CO absorption may be the normal state of the spectrum, and that atmospheric absorption is masked by strong, circumstellar emission associated with the onset of a sudden burst of outflow activity. In our more recent spectra, both sources again show CO (and \(H\) i) in absorption. However, like Hrivnak et al., we do not detect \(H_2\) emission lines in either of these PPN, so we do not present the spectra here. Notably, unlike many other PPN that emit in CO, Bujarrabal et al. (2001) find no sign of high-velocity line wings in their millimetre-wave spectra of either source. This lack of high-velocity molecular gas may be related to the absence of detectable (shock-excited) \(H_2\) in our spectra.

3.2 Planetary nebulae

3.2.1 NGC 6302 and 6537

NGC 6302 and 6537 are very high-excitation PN (Kaler 1986; Rowlands, Houck & Herter 1994; Pottasch et al. 1996; Casassus, Roche & Barlow 2000; Feibelman 2001); in both nebulae emission lines from [Ne v] and [Si vi] have been observed, ions that require photons with energies \(\sim 100–200\) eV to form. Both objects therefore...
could be due to a combination of shocks and photoionization by the central star in each system (Rowlands et al. 1994; Feibelman 2001). In NGC 6302, P Cygni profiles detected in the highly ionized species point to stellar winds with velocities of 300–700 km s\(^{-1}\) (Feibelman 2001), while nebula expansion velocities of the order of 300 km s\(^{-1}\) have been reported for NGC 6537 (Corradi & Schwartz 1993; Cuesta, Phillips &amp; Mampaso 1995). Both nebulae also exhibit strong polycyclic aromatic hydrocarbon (PAH) emission (Roche et al. 1996).

Kastner et al. (1996) imaged both nebulae in H\(_2\) emission. Like them, we detect H\(_2\) emission along the limb-brightened edges of each extended, bipolar nebula, and around the central high-excitation regions (Figs 1c and d). In the continuum-subtracted image of NGC 6302 in Fig. 2 the H\(_2\) emission in the core appears to be confined to an equatorial ring (diameter \(\sim\)10 arcsec; centred at offset 0, 0 arcsec) that is elongated north–south. Our spectrograph slit was centred on the bright continuum peak in NGC 6302 and orientated east–west, so that emission from this ring and the extended bipolar lobes was observed. In NGC 6537 the H\(_2\) is likewise excited in a ring around the central highly ionized core (Fig. 2). Unfortunately, in NGC 6537 our slit was positioned across the central region only; it did not pass through any of the emission filaments in the extended bipolar lobes.

Spectra at various locations in NGC 6302 and 6537 are presented in Figs 8 and 9. In NGC 6302 the top spectrum and bottom two spectra (positions ‘up2’, ‘dn2’ and ‘dn3’) correspond to regions in the filamentary bipolar lobes, while the other three spectra derive from the bright core. In NGC 6537 spectra at three locations across the core are presented. Br\(\gamma\) emission dominates in the core regions in both sources, as one would expect for these high-excitation nebulae. In NGC 6302 the H\(_2\) 1–0 S(1) emission line begins to dominate in the limb-brightened lobes.

We also detect Br\(\delta\) at 1.944 \(\mu\)m, He i (2.058 and 2.122 \(\mu\)m), He ii (2.189 \(\mu\)m) and [Fe iii] (2.347 \(\mu\)m) in the central regions in each nebula; i.e. in all three spectra in NGC 6537 (Fig. 9) and in the central three spectra in NGC 6302 (Fig. 8). These are expected in high-excitation PN (see, e.g., Hubble 12; Ramsay et al. 1993).

### 3.2.2 NGC 6886 and Hb 5

NGC 6886 is moderately evolved (perhaps 10 000 yr post-AGB) and, like NGC 6302 and 6537, it is a high-excitation PN (Aller &amp; Czyzak 1979; Hyung, Keyes &amp; Aller 1995). Weinberger (1989) and Taylor, Gussie &amp; Pottasch (1990) report expansion velocities of 20–25 km s\(^{-1}\) for the ionized and atomic gas in the nebula. Like NGC 6302 and 6537 (and Hb 5 discussed below) NGC 6886 also has strong PAH emission in the near-IR (Magazzu &amp; Strazzulla 1992; Roche et al. 1996). The compact size of this nebula is probably due to its distance (up to 6 kpc has been reported in the literature), its youth, or a combination of both (Hyung et al. 1995). Indeed, in our near-IR images we only detect emission from a compact nebula. In Fig. 1(e) the nebula appears to be circular, though with a possible layer of obscuration across its centre, orientated NW–SE. This ‘dark lane’ seems to extend over approximately 10 arcsec, producing a faint ring in this NW–SE direction. The continuum-subtracted image in Fig. 2 shows that the H\(_2\) is confined to the arcs or shells along the orthogonal NE–SW axis.

Hb 5 is a moderate-excitation bipolar PN that, in optical images, extends over an arcmin on the sky, in an ENE–WSW direction. The two bubble-like lobes of this nebula exhibit remarkable point-symmetry (Corradi &amp; Schwartz 1993, 1995). High nebula expansion velocities of approximately 250 km s\(^{-1}\) have been observed in the ionized gas in these extensive bipolar lobes (Corradi &amp; Schwartz 1993; Pishmish, Manteiga &amp; Recio 2000). Consideration of the source morphology and kinematics suggest that Hb 5 may be less evolved than the more fragmented nebulae associated with NGC 6537 and 6302 (Corradi &amp; Schwartz 1993), though Hb 5...
C. J. Davis et al.

Figure 9. Spectra were extracted from three central regions in the PN NGC 6537; from top-to-bottom, the spectra are from the up, cen and dn regions labelled in Fig. 1(d). See Fig. 8 for a description of line identifications.

Figure 10. H$_2$ was only observed in the central core in the PN NGC 6886, though the emission is slightly extended, so three spectra are presented – from top-to-bottom the spectra are from the up, cen and dn areas illustrated in Fig. 1(e). See Fig. 8 for a description of line identifications.

Figure 11. H$_2$ emission was only detected toward the bright core region of the PN Hb 5; nevertheless, spectra at three locations in this central region are presented. From top-to-bottom the spectra represent areas up, cen, dn (as labelled in Fig. 1(f)). See Fig. 8 for a description of line identifications.

is probably more evolved than NGC 6886. In our near-IR images of Hb 5 (Fig. 1f) we detect H$_2$ emission predominantly from the bright core (see also Kastner et al. 1996); our continuum-subtracted image in Fig. 2 only hints at possible filamentary H$_2$ emission in the bipolar lobes (a deeper image is needed to confirm these features). The emission in the core is complex and clumpy; overall, the emission is roughly cross-shaped, so it may be associated with the limb-brightened cavity walls of the bipolar lobes seen in the optical range.

K-band spectra at three locations across the NGC 6886 and Hb 5 nebulae are presented in Figs 10 and 11. As well as H$_2$ emission lines, He I lines at 2.058 and 2.112 µm (the latter is close to, though still resolved from, the H$_2$ 1–0 S(1) line), He II at 2.189 µm and [Fe III] at 2.347 µm are again evident in all spectra across both sources. Br$\gamma$ at 1.944 µm is also detected in NGC 6886 and Hb 5; the Br$\gamma$/Br$\delta$ ratio in the former measures 1.4–1.6, while in the latter, ratios of 2.1–2.6 are measured. These are consistent with reddened, ionized nebula (Br$\gamma$/Br$\delta$ $\sim$ 1.4 for $T_e$ $\sim$ 10$^4$ K).

3.2.3 NGC 6445

Although it appears morphologically similar to NGC 7048 in Fig. 1, NGC 6445 is, in fact, more akin to the high-excitation PN NGC 6302 and NGC 6537 (Corradi & Schwartz 1995; van Hoof et al. 2000). Of the three PN, the NGC 6445 nebula has a somewhat lower temperature and density, and is probably the older, more evolved source (Pottasch, Beintema & Feibelman 2000; van Hoof et al. 2000). In optical images the nebula comprises an inner, $\sim$40-arcsec diameter ring which is enclosed by a much larger, though fainter bipolar nebula orientated at a PA $\sim$75$^\circ$ (Corradi & Schwartz 1995; Zhang & Kwok 1998). H$_2$ emission is predominantly observed in the

NIR spectroscopy of (proto)-planetary nebulae

3.2.4 NGC 7048

NGC 7048 is an extensive, evolved PN that was shown to be bright in H$_2$ emission by Kastner et al. (1996). Zhang & Kwok (1998) model early optical images of this nebula with an ‘ellipsoidal shell’ model and identify NGC 7048 as an elliptical PN. Our new near-

4 ANALYSIS OF THE H$_2$ DATA

4.1 Line ratios, excitation and the H$_2$ ortho–para ratio

The simplest way to analyse the data set described above is by considering various line ratios. We list a number of useful ratios in Table 3. All line ratios are extinction-corrected, using a $K$-band...
Table 3. Line intensity ratios (corrected for extinction) derived from H$_2$ 1–0 S(1), 2–1 S(1) and 3–2 S(3) lines (at 2.121, 2.247 and 2.201 μm), Brγ (at 2.166 μm) and He I (at 2.058 μm).

<table>
<thead>
<tr>
<th>Target</th>
<th>$A_4^2$</th>
<th>1–0 S(1)/2–1 S(1)</th>
<th>1–0 S(1)/3–2 S(3)</th>
<th>1–0 S(1)/Brγ</th>
<th>1–0 S(1)/He I</th>
<th>$\phi_1^3$</th>
<th>$\phi_2^5$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PPN (and young PN):</strong></td>
<td></td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CRL 2688 (jet)</td>
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<td></td>
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</tr>
<tr>
<td>- jup</td>
<td>1.8</td>
<td>5.2 (±0.5)</td>
<td>&gt;26</td>
<td>–</td>
<td>&gt;32</td>
<td>3.3</td>
<td>–</td>
</tr>
<tr>
<td>- jdn</td>
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<td>8.4 (±1.0)</td>
<td>&gt;45</td>
<td>–</td>
<td>&gt;40</td>
<td>3.2</td>
<td>2.9</td>
</tr>
<tr>
<td>CRL 2688 (disc)</td>
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</tr>
<tr>
<td>- dup2</td>
<td>2.0</td>
<td>10.1 (±0.4)</td>
<td>58 (±9)</td>
<td>&gt;200</td>
<td>&gt;500</td>
<td>3.2</td>
<td>3.4</td>
</tr>
<tr>
<td>- dup</td>
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<td>13.5 (±3.0)</td>
<td>&gt;41</td>
<td>&gt;45</td>
<td>&gt;200</td>
<td>3.1</td>
<td>–</td>
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<td>–</td>
<td>–</td>
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<td>–</td>
<td>–</td>
</tr>
<tr>
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<td>2.1</td>
<td>10.2 (±0.6)</td>
<td>44 (±13)</td>
<td>&gt;400</td>
<td>&gt;400</td>
<td>3.1</td>
<td>3.0</td>
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<td>–</td>
<td>–</td>
<td>3.8 (±0.4)</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>- dn</td>
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<td>–</td>
<td>–</td>
<td>1.4 (±0.4)</td>
<td>–</td>
<td>–</td>
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<td></td>
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</tr>
<tr>
<td>- up</td>
<td>1.7</td>
<td>6.1 (±0.8)</td>
<td>&gt;14</td>
<td>&gt;28</td>
<td>&gt;10</td>
<td>3.0</td>
<td>–</td>
</tr>
<tr>
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<td>–</td>
<td>–</td>
<td>0.24 (±0.1)</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>- dn</td>
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<td>6.6 (±1.6)</td>
<td>&gt;10</td>
<td>&gt;17</td>
<td>&gt;5</td>
<td>3.0</td>
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</tr>
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<td>- cen</td>
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<td>5.0 (±1.5)</td>
<td>20 (±8)</td>
<td>1.2 (±0.1)</td>
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<td>2.4</td>
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</tr>
<tr>
<td>- cen</td>
<td>2.0</td>
<td>4.2 (±1.5)</td>
<td>&gt;10</td>
<td>0.8 (±0.1)</td>
<td>2.1 (±0.5)</td>
<td>3.0</td>
<td>–</td>
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<tr>
<td>- up2</td>
<td>2.5</td>
<td>3.5 (±0.9)</td>
<td>–</td>
<td>1.3 (±0.2)</td>
<td>2.5 (±0.4)</td>
<td>2.7</td>
<td>–</td>
</tr>
<tr>
<td>- up</td>
<td>0.5</td>
<td>3.2 (±0.7)</td>
<td>7.5 (±2.3)</td>
<td>0.16 (±0.04)</td>
<td>0.20 (±0.01)</td>
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<td>–</td>
</tr>
<tr>
<td>- cen</td>
<td>2.4</td>
<td>6.7 (±1.4)</td>
<td>&gt;12</td>
<td>0.10 (±0.01)</td>
<td>0.19 (±0.01)</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>- dn</td>
<td>2.0</td>
<td>3.9 (±0.6)</td>
<td>&gt;11.5</td>
<td>0.14 (±0.01)</td>
<td>0.22 (±0.01)</td>
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<tr>
<td>- dn2</td>
<td>2.2</td>
<td>2.1 (±0.8)</td>
<td>&gt;7</td>
<td>0.6 (±0.1)</td>
<td>1.0 (±0.2)</td>
<td>–</td>
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<tr>
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<td>12.6 (±2.0)</td>
<td>–</td>
<td>3.9 (±0.4)</td>
<td>4.3 (±0.5)</td>
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<td>- up</td>
<td>3.1</td>
<td>4.2 (±1.8)</td>
<td>–</td>
<td>0.14 (±0.01)</td>
<td>0.38 (±0.02)</td>
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<td>0.6</td>
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<tr>
<td>- cen</td>
<td>2.3</td>
<td>8.4 (±2.5)</td>
<td>&gt;11</td>
<td>0.10 (±0.01)</td>
<td>0.32 (±0.01)</td>
<td>2.3</td>
<td>0.9</td>
</tr>
<tr>
<td>- dn</td>
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<td>4.0 (±1.8)</td>
<td>–</td>
<td>0.13 (±0.01)</td>
<td>0.33 (±0.02)</td>
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<tr>
<td>- up</td>
<td>1.4</td>
<td>6.1 (±0.6)</td>
<td>–</td>
<td>0.17 (±0.01)</td>
<td>0.56 (±0.03)</td>
<td>2.5</td>
<td>1.2</td>
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<tr>
<td>- cen</td>
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<td>10.5 (±2.0)</td>
<td>–</td>
<td>0.11 (±0.01)</td>
<td>0.38 (±0.03)</td>
<td>2.5</td>
<td>2.7</td>
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<tr>
<td>- dn</td>
<td>0.6</td>
<td>5.8 (±0.5)</td>
<td>–</td>
<td>0.17 (±0.01)</td>
<td>0.50 (±0.03)</td>
<td>2.4</td>
<td>0.6</td>
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<tr>
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</tr>
<tr>
<td>- up</td>
<td>0</td>
<td>13.1 (±2.0)</td>
<td>17 (±8)</td>
<td>0.15 (±0.01)</td>
<td>0.56 (±0.01)</td>
<td>1.8</td>
<td>–</td>
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<tr>
<td>- cen</td>
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<td>2.6 (±1.0)</td>
<td>&gt;5</td>
<td>0.10 (±0.01)</td>
<td>0.36 (±0.01)</td>
<td>2.4</td>
<td>–</td>
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<tr>
<td>- dn</td>
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<td>12.2 (±2.0)</td>
<td>18 (±6)</td>
<td>0.27 (±0.01)</td>
<td>0.71 (±0.02)</td>
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<tr>
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<td>1.3</td>
<td>10.2 (±2.0)</td>
<td>24 (±2)</td>
<td>2.0 (±0.1)</td>
<td>7.5 (±1.0)</td>
<td>3.1</td>
<td>1.4</td>
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<tr>
<td>- cen</td>
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<td>8.3 (±3.0)</td>
<td>13 (±6)</td>
<td>1.2 (±0.1)</td>
<td>4.9 (±0.3)</td>
<td>2.8</td>
<td>1.2</td>
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<tr>
<td>- dn</td>
<td>–</td>
<td>–</td>
<td>–</td>
<td>0.37 (±0.02)</td>
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<tr>
<td>- dn2</td>
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<td>9.8 (±1.0)</td>
<td>13 (±2)</td>
<td>1.4 (±0.1)</td>
<td>4.1 (±0.5)</td>
<td>3.0</td>
<td>1.6</td>
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</tr>
<tr>
<td>- up2</td>
<td>1.7</td>
<td>19.2 (±2.4)</td>
<td>&gt;38</td>
<td>15 (±6)</td>
<td>21 (±9)</td>
<td>2.8</td>
<td>0.8</td>
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<tr>
<td>- up</td>
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<td>12.7 (±2.0)</td>
<td>&gt;21</td>
<td>13 (±3)</td>
<td>30 (±10)</td>
<td>2.9</td>
<td>1.6</td>
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<tr>
<td>- cen</td>
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<td>12.3 (±1.8)</td>
<td>–</td>
<td>10 (±1.8)</td>
<td>12 (±3)</td>
<td>2.2</td>
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<tr>
<td>- dn</td>
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<td>20.0 (±2.5)</td>
<td>&gt;44</td>
<td>18 (±3)</td>
<td>37 (±15)</td>
<td>3.3</td>
<td>1.5</td>
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<td>10.4 (±1.9)</td>
<td>–</td>
<td>8.7 (±1.8)</td>
<td>19 (±5)</td>
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<td>- dn3</td>
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<td>&gt;39</td>
<td>26 (±2)</td>
<td>14 (±2)</td>
<td>3.0</td>
<td>1.2</td>
</tr>
</tbody>
</table>

1See Fig. 1 for the spatial position on each target (up, cen, dn, etc.).
2$K$-band extinction, measured from the 1–0 S(1)/1–0 Q(3) line ratio. A dash indicates that no measurement was possible because of the non-detection of H$_2$. A zero indicates a line ratio consistent (to within the errors) with no reddening.
3The H$_2$ ortho–para ratio. The $v = 1$ values ($\phi_1$) are derived from the 1–0 S(0), 1–0 S(1) and 1–0 S(2) integrated line intensities (at 2.223, 2.121 and 2.033 μm), while the $v = 2$ values ($\phi_2$) are estimated from the 2–1 S(1), 2–1 S(2) and 2–1 S(3) intensities (at 2.247, 2.154 and 2.073 μm), following the method derived by Smith et al. (1997).
extinction estimate derived from the ratio of the H$_2$ 1–0 S(1) and 1–0 Q(3) lines. Since both lines arise from the $v = 1$, $J = 3$ rotational level, the intrinsic flux ratio is fixed and can only take a different value through differential extinction. We adopt an extinction law of the form $\lambda^{-1.7}$, so that measured line ratios (for lines at $\lambda_1$ and $\lambda_2$) are modified by the factor: $10^{0.4k_{H_2}(\lambda_2/\lambda_1)^{1.7-1}}$, where $\lambda = 2.2$ $\mu$m and $A_2$ is the extinction at 2.2 $\mu$m. The Q(3) line occurs in a relative poor part of the K-band atmospheric window, however, so $A_2$ is to some degree uncertain. Fortunately, the derived extinction values are in all cases relatively low, and the observed lines are closely spaced in wavelength, so the extinction values used will introduce an uncertainty of at most 20 per cent to the line ratios listed. This uncertainty is in addition to the errors given in Table 3.

The H$_2$ 1–0 S(1)/2–1 S(1) ratio has on occasion been used to distinguish thermal from non-thermal excitation, although for densities above $10^4$ cm$^{-3}$ collisional de-excitation of FUV-pumped molecules will thermalize the lower-energy states and thereby yield line ratios typical of gas in local thermodynamic equilibrium (LTE) (Burton, Hollenbach & Tielens 1990; Hollenbach & Natta 1995). The higher vibrational states are expected to retain a fluorescent population, however. For example, the PDR models of Hollenbach & Natta (1995) predict 1–0 S(1)/2–1 S(1) ratios of 2 or 3 for densities of the order of $10^3$–$10^4$ cm$^{-3}$, with the ratio increasing to 10–20 for densities of $10^4$–$10^6$ cm$^{-3}$. Similarly high ratios are predicted from thermally excited gas and gas in the hot, dense regions behind molecular shocks (e.g. Smith 1995). Conversely, the 1–0 S(3)/3–2 S(3) ratio retains a value of approximately 8 in a dense PDR ($n_H = 10^3$–$10^4$ cm$^{-3}$, for a flux of $\sim 10^3 G_{0}$, where $G_{0}$ is the average interstellar radiation field; Burton et al. 1990). Only for very high densities and very intense FUV radiation fields ($n_H = 10^7$–$10^8$ cm$^{-3}$, FUV flux $\geq 10^3 G_{0}$) will this ratio approach a thermal or ‘shock’ value of 10–100. The combination of the 1–0 S(1)/2–1 S(1) and 1–0 S(1)/3–2 S(3) ratios should therefore give some indication as to the excitation of the H$_2$ in each (P)PN.

It is interesting to note in Table 3 that the highest ratios are measured in the young PPN, CRL 2688 and in the most evolved source in our sample, NGC 7048. These data suggest that thermal excitation dominates, with little contribution from FUV excitation. Progressively lower ratios are measured in the intermediate-stage objects, where values typical of PDRs are observed (e.g. Dinerstein et al. 1988;Hora & Latter 1994; Shupe et al. 1998). In Hb 5, for example, relatively high 1–0 S(1)/2–1 S(1) ratios are measured in the ‘up’ and ‘dn’ positions, but the 1–0 S(1)/3–2 S(3) ratios are relatively low. The ‘thermal’ excitation suggested by the former is not supported by the latter. Instead, the gas is probably excited in a high-density PDR. In Hb 5 and in other objects we also see line ratios that change across the region, reflecting the changing physical conditions. In NGC 6537 and 6886, for example, the 1–0 S(1)/2–1 S(1) ratio is markedly high in the core region, though lower further out (in the ‘up’ and ‘dn’ positions). Again, thermalization of fluoresced gas probably explains this trend, rather than the presence of shocks.

In Table 3 we also list the H$_2$ 1–0 S(1)/Br$\gamma$ and H$_2$ 1–0 S(1)/He $\lambda$ 2$P$–2$S$(2.058 $\mu$m) line ratios. The former is highest in the least and most evolved sources in our sample (where H$_2$ is detected). The high H$_2$ 1–0 S(1)/Br$\gamma$ ratio in NGC 7048 can be understood in terms of shock excitation of H$_2$ in the expelled AGB envelope (which is now at some distance from the faint CSPN) producing bright H$_2$ lines, with weak Br$\gamma$ emission from the distended, ionized ‘bubble’ that separates the H$_2$-bright rings from the CSPN. In the less-evolved PN the H II region surrounding each CSPN is more compact, the emission measure is higher and so the H$_2$/Br$\gamma$ line ratio is lower. In most sources we also see a clear indication of a lower ratio toward the centre of the region.

Guerrero et al. (2000) suggest that the H$_2$ 1–0 S(1)/Br$\gamma$ ratio should correlate with the evolutionary stage and bipolarity of each PN. They suggest that small, bipolar nebulae have low ratios (less than unity), while evolved PN with large, well-defined rings and bright central stars have larger ratios. Similarly, the models of Natta & Hollenbach (1998) suggest a high ratio for high-mass cores and/or evolved sources. Our PN data generally support these ideas, although of course the correlation with age does not extend to the PPN phase. We find that, overall, the highest H$_2$ 1–0 S(1)/Br$\gamma$ ratios are observed toward the sources with H$_2$ 1–0 S(1)/2–1 S(1) and 1–0 S(1)/3–2 S(3) ratios consistent with thermal and probably shock excitation (see also García-Hernández et al. 2002).

Photionization of atomic helium (by photons with energies $>24.6$ eV), followed by recombination and cascade to the 2$S$ triplet state and then electronic collisional de-excitation to the 2$P$ singlet level will yield 2.058-$\mu$m emission in PN, given sufficiently high densities ($n_{\text{nit}} \sim 4 \times 10^4$ cm$^{-3}$ for the collisional transition between the 2$S$ and 2$P$ states). Consequently, the H$_2$ 1–0 S(1)/He $\lambda$ 2$P$–2$S$ ratio in Table 3 will, like the H$_2$ 1–0 S(1)/Br$\gamma$ ratio, distinguish high-excitation objects from their lower-excitation, molecular counterparts. Indeed, the H$_2$ 1–0 S(1)/He $\lambda$ 2$P$–2$S$ ratio closely follows the H$_2$ 1–0 S(1)/Br$\gamma$ ratio, once again peaking in the youngest targets and in the most evolved PN in our sample, and matching the changing excitation across each object as traced by the H$_2$ 1–0 S(1)/Br$\gamma$ ratio.

Finally, from the 1–0 S(1), 1–0 S(2) and 1–0 S(3) line intensities we measure the ortho–para ratio for the $v = 1$ states, $\phi_v$, following the technique described by Smith, Davis & Lioure (1997). In a similar way, a ratio for the $v = 2$ states is calculated for a few locations (see below). The method benefits from the fact that the three transitions are close in wavelength, so that derived values for $\phi_v$ are relatively insensitive to extinction, and the transitions have upper states that are populated at essentially the same rotational excitation temperature.

H$_2$ is formed on warm dust grains with a ratio of 3:1, this being the ratio of the statistical weights of the nuclear spins (aligned/opposed spins). For gas in LTE at temperatures above $\sim 200$ K the H$_2$ retains this ratio. In lower-temperature gas, a lower ratio would eventually result, although the conversion may be slow (Burton, Hollenbach & Tielens 1992) and bright H$_2$ emission is unlikely to be produced. In PDRs, low ratios are also predicted, not because of a true ortho–para abundance ratio of less than 3 (Sterberg & Neufeld 1999) but because of the preferential pumping of the para states across a layer of self-shielding gas (these states have a higher opacity to FUV photons than the ortho states). Indeed, ratios in the range 1.5–2.2 have been measured, especially for the higher-energy vibrational states (e.g. Ramsay et al. 1993; Lumsden et al. 2001). Note, however, that the actual (total) ortho–para ratio may still be close to an equilibrium value near 3.

In Table 3 we list the $v = 1$ ortho–para ratio for each source and each extracted spectrum. Again we see a subtle change in $\phi_v$ with source evolution. The highest values ($\sim 3$, consistent with shocks or thermalization of the $v = 1$ levels) are measured in the least and most evolved sources in our sample, CRL 2688 and NGC 7048 (excluding the early post-AGB sources where H$_2$ was not detected). Slightly lower values, of around $2.5$, are measured in the intermediate objects; this again suggests that fluorescence is more important in these targets. The very low values for $\phi_v$ measured in some PDRs, such as Hubble 12 (Ramsay et al. 1993 report $\phi = 2.1$) are not observed.
in any of our targets, so some shock reprocessing or thermalization must be occurring, even in the intermediate-stage PN. Overall, the values for the PN in Table 3 are consistent with measurements made in other, similar sources (e.g. Hora et al. 1999; Lumsden et al. 2001).

The derived ortho–para ratios $\phi_1$ in Table 3 are of course applicable only to the $v = 1$ levels, so they do not tell the whole story. In a few cases, a value for the $v = 2$ levels is derived from the $2\rightarrow 1$ S(1), 2–1 S(2) and 2–1 S(3) transitions [the 2–1 S(0) line was not used since this lies near the red end of the K-band]. The ratio from these transitions is given by (Smith et al. 1997)

$$1/\phi_2 = 0.898(L_2/L_1)^{0.448}(L_2/L_1)^{0.552}.$$  

(1)

[Note that the above equation yields the reciprocal of $\phi_2$ because the S(1), S(2) and S(3) lines are used instead of the S(0), S(1) and S(2) lines.]

Although the values for $\phi_2$ are less certain than the values for $\phi_1$ [the $v = 2$ transitions are of course weaker than the $v = 1$ lines, and the S(2) line is close to (and sometimes blended with) the Br$\gamma$ line], the results in Table 3 nevertheless again indicate a trend for lower ortho–para ratios in the intermediate objects with higher values in CRL 2688. NGC 7048, the evolved PN with line

4.2 The CDR method

A more sophisticated way of analysing the H$_2$ excitation is via the column density ratio method, as described, for example, by Burton & Haas (1997) and Eisloffel, Smith & Davis (2000). We use this method to test whether a shock+fluorescent combination can be used to adequately model the observed line intensities. This model is preferred over a high-density fluorescence model for the reasons described in the introduction.

Having extracted all of the available H$_2$ line fluxes, we determine the columns of gas needed to produce the integrated fluxes and plot these data on to CDR diagrams in Figs 14–18. We then use these data to derive the following four quantities.

(i) The relative fluorescent and shock contributions to the gas excitation, $f_{\text{flu}}$.
(ii) The shock excitation temperature, $T_s$.
(iii) The H$_2$ ortho–para ratio for the fluorescent component of the gas (the overall ratio may still be close to 3).
(iv) The average extinction.

First, as noted earlier we calculate the extinction (where possible) from the 1–0 S(1) and 1–0 Q(3) lines assuming a power-law extinction relation of the form $I_{\nu} \propto \nu^{-1.7}$. The relative extinction is then applied to the measured fluxes before the modelling commences.

Secondly, to identify the underlying physical processes, we calculate the column density in the upper energy level for each observed H$_2$ transition. When in local thermodynamic equilibrium, the column density, $N_j$, of the energy level $kT_j$ is proportional to the level degeneracy, $g_j$, and the factor $\exp(-T_j/T)$. We normalize the column to the column for the level $v = 1$, $J = 3$, corresponding to the 1–0 S(1) line, and define this as the column density ratio.

The exponential dependence on $T_j$ renders plots of log(CDR) versus $T_j$ largely uninformative. We therefore display a ‘normalized’ column density ratio, CDR/CDR(2000 K), where the constant CDR(2000 K) = $\exp(-T_j + 6953 K)/2000$ K. This eliminates the exponential factor provided the gas temperature is of the order of 2000 K, permitting accurate modelling. In such diagrams, a horizontal straight line with log[CDR/CDR(2000 K)] = 0 represents 2000 K gas in LTE, a sloping straight line represents LTE gas at a

Figure 14. CDR diagrams for the six spectra observed in the PPN CRL 2688. The positions are labelled in Fig. 1; the spectra themselves are shown in Fig. 3. Data points are plotted as boxes (with error bars) except for columns derived from the 1–0 Q-branch lines which are plotted as crosses. The full and dashed lines represent pure-shock model fits to the $v = 1$ and $v > 1$ data, respectively (we approximate the non-LTE conditions by fitting these data separately). The diamonds represent the final shock+fluorescent model fits to the data. The shock models assume an ortho–para ratio of 3; the additional flux predicted by the PDR model 14 of Black & van Dishoeck (1987) is modified by the ortho–para H$_2$ ratio, ‘op’, given in each plot (see the text for details). As is the extinction correction applied to the data, derived from the 1–0 S(1)/1–0 Q(3) line ratio; $T_r$ is the rotational temperature for the $v = 1$ states in the shocked gas.

temperature other than 2000 K, and a curve represents a range of temperatures (as expected, say, from a curved shock surface).

Thirdly, we fit shock models to the CDR data points. A range of models has been calculated, employing J-type and C-type shocks in planar and curved shock configurations. Details of the shock codes employed are presented by Eislöffel et al. (2000) and described by Smith et al. (2003). To approximate the non-LTE conditions expected in each target we predict two shock CDR curves, one for the first vibrational level (drawn with a full curve) and a second for the higher-energy states (the dashed curves). Note that, with lower gas densities the higher vibrational levels become radiatively (rather than collisionally) depopulated. This is distinguishable from fluorescence because fluorescence greatly overpopulates the higher vibrational levels, while non-LTE excitation should underpopulate these levels. However, as we describe below, the degree to which fluorescence contributes varies, from source to source and spatially across targets that are resolved.

We find that the shock models generally provide no more than a rough fit because there is a dominant fluorescent contribution to all but the columns belonging to the first vibrational level; i.e. for \( v > 1 \) the CDR values are generally situated above the shock-model curves. This is also recognizable by the non-linear distribution of the CDRs from the rotational levels within each vibrational level. In other words, the CDR values appear scattered on each diagram, rather than being on a single, smooth curve, as is often the case in purely shock-excited sources such as Herbig—Haro objects (e.g. Burton & Haas 1997; Davis et al. 1999; Eislöffel et al. 2000). It is clear that for most of the (P)PN considered, a pure shock model fails to account for the \( \text{H}_2 \) population.

We therefore superimpose an ultraviolet (UV) fluorescent component and lower the shock contribution (or choose a lower excitation shock) until a plausible fit is uncovered. We chose the fluorescent model tabulated by Black & van Dishoek (1987) (model 14) which assumes moderate gas densities \( n_{\text{H}} = 3 \times 10^5 \text{ cm}^{-3} \) and a low gas temperature (100 K). The incident UV flux therefore yields a non-thermal fluorescent spectrum. An ortho—para ratio for radiatively excited \( \text{H}_2 \) of \( \phi = 1.7 \) was found in model 14 (ortho—para ratio = 3 in our shock models). However, to improve our fit we have adjusted the fluxes from the para \( \text{H}_2 \) levels predicted by model 14 by a factor of \( 1.7/\phi \), where a value of \( \phi \) which gives the best fit to the relative rotational distributions is chosen. The value of \( \phi \) used in each case is displayed in each plot (referred to as ‘\( \phi' \)). Note that this ortho—para ratio applies only to the fluorescent contribution to the line fluxes: the ortho—para ratios listed in Table 3 for the \( v = 1 \) transitions (\( \phi_1 \)) differ markedly; only the (\( \phi_2 \)) values are expected to be similar to the values derived from the CDR modelling. The fitting procedure is manual in the sense that line measurements that seem to be spurious are not considered. In this way the best quality data (points with the lowest errors) at each location are modelled. The final shock plus-fluorescence combination, plotted with diamond symbols in Figs 14–18, can be unique to each source and to each position across each source, provided sufficient data from various vibrational levels are available.

The fluorescent contribution indicated in each panel as \( f_{\text{flu}} \) is defined as the ratio of the fluorescent to the shock flux in the 1–0 S(1) line. Fluorescence will, of course, contribute an increasingly higher fraction to the columns of the higher vibrational levels.

Finally, a rotational excitation temperature for the shocked gas, \( T_r \), is derivable provided fluorescence makes a low contribution to the columns of the first vibrational level (so that these low-energy states are thermally populated in the shock). The excitation temperature is most accurately obtained from the 1–0 S(3)/1–0 S(1) ratio using the standard formula (Eislöffel et al. 2000). The values derived from the S(1)/S(3) ratio predicted by the shock model component of the overall shock+fluorescence fit to the data are shown directly on the figures.


Figure 15. CDR diagrams for the spectra observed in two other PPN, M 1-92 and IRAS 17150–3224, and in two ‘young’ PN, IRAS 18062+2410 and 21282+5050. The separate positions in M 1-92 and IRAS17150–3224 are labelled in Fig. 1; the spectra themselves are shown in Figs 4–7. See Fig. 14 for a description of the symbols used. Note that the model for M 1-92-dn demonstrates consistency with M 1-92-up rather than an independent determination of model parameters.
4.3 H₂ excitation in PPN and PN

As a measure of the relative importance of shock and fluorescent excitation we discuss the derived values for $f_{lu}$ and the rotational excitation temperature, $T_r$, across each source.

4.3.1 The PPN

The CDR diagrams at positions across three PPN are shown in Figs 14 and 15. For CRL2688, our most complete data set, the excitation in the bipolar lobes and equatorial plane are analysed separately; spatial variations in some of the derived parameters are also shown in Fig. 19. CRL 2688 is one of the least-evolved sources in our sample. Previous excitation studies, and the line ratio analysis presented in Section 4.1, indicate that shock excitation dominates in this object. Our CDR analysis generally confirms this finding. The $v = 1$ CDRs are reasonably well fitted by the pure shock model (the solid line), and the ratio of fluorescence to shock excitation predicted by the model fits is very low at all positions, in both the equatorial plane and the bipolar lobes. The ortho–para H₂ ratios derived from the $v = 1$ and $v = 2$ transitions (listed in Table 3 and displayed in Fig. 19) are also consistently high in CRL 2688. We do see a slight increase to the fluorescent contribution in the most central spectrum (crl 2688-dcen), and an associated drop in the rotational excitation temperature (Fig. 19), though this is based on weak emission lines and the detection of only one high-excitation H₂ line.

M 1-92 and IRAS 17150–3224 are two similar bipolar PPN, though weak Brγ is detected in both sources (in the latter Brγ dominates near the CSPN, while H₂ is strongest in the bipolar lobes): these two objects may be somewhat more evolved than CRL 2688. Higher-quality data are required for M1-92 before a proper analysis is possible. However, sufficient lines were detected in the bipolar lobes in IRAS 17150–3224. In comparison to CRL 2688, the CDR fits in Fig. 15 suggest that a slightly higher (though still relatively modest) fluorescent contribution to the molecular gas excitation is needed to explain the populations of the higher-energy states. The presence of this non-thermal excitation mechanism is supported by the lower rotation temperatures predicted for the $v = 1$ CDRs and the lower H₂ line ratios in Table 3.

4.3.2 The ‘young’ PN

The CDR data for IRAS 18062+2410 and 21282+5050 are also shown in Fig. 15. These sources are probably slightly more evolved than CRL 2688, M 1-92 and IRAS 17150–3224 and are recognized as young PN rather than PPN. In both objects Brγ is as bright as the H₂ 1–0 S(1) line. In IRAS 18062+2410 a number
of high-excitation lines have been detected and fluorescence now makes a more significant contribution to the excitation of the \( v = 1 \) lines, and the higher-energy states (Fig. 15 and Table 3). In IRAS 21282+5050 shocks again seem to dominate the excitation (note the lack of higher-excitation lines in Figs 7 and 15), though in these marginal data fluorescence may still be important. Higher gas densities in IRAS 21282+5050 may account for the higher excitation temperatures; the fact that the full and dashed lines in the pure-shock models join in Fig. 15 (for IRAS 21282+5050) also point to conditions approaching LTE. Notably, in both cases the 1–0 S(1)/2–1 S(1) ratios in Table 3 are low (‘non-thermal’).

The underlying trend, therefore, appears to be for an increasing fluorescent contribution to the molecular gas excitation with PPN-to-young-PN evolution. The data are also consistent with shock excitation, as measured by the rotational excitation temperature, \( T_r \), decreasing.

### 4.3.3 The more evolved PN

CDR plots for the higher-ionization PN are presented in Figs 16 and 17. The lack of higher-excitation (\( v > 1 \)) line emission in NGC 6302 precludes a good fit for the shock+fluorescence model, although \( f_{\text{flu}} \) is still marginally higher in these targets than in the PPN. In NGC 6302 \( f_{\text{flu}} \) is somewhat higher in the central regions than it is in the extended filamentary wings, positions ‘up2’ and ‘dn3’ where the shocks are likely to dominate (see also Fig. 19). In NGC 6537 spectra from only the central region are analysed; here, fluorescence is again important, though high excitation temperatures are also notable.

The PN NGC 6886, Hb 5 and NGC 6445 are associated with ionized nebula (as demonstrated by the He II and [Fe II] emission lines in our spectra). In each case the post-AGB envelope is fully detached from the CSPN and may have been driven some distance from the central star. Nevertheless, fluorescent and shock excitation again both contribute to the molecular gas excitation, with the former again being most important in the inner, core regions (in Hb 5; cen position) and along the inner edges of the expanding, post-AGB dust shell (in NGC 6445-cen). Note also in Table 3 that \( \phi_1 \) and particularly \( \phi_2 \) are low throughout.

Finally, in probably our most evolved PN, NGC 7048, only very weak nebula emission lines are detected. We detect H\(_2\) emission from the molecular shell, where shock excitation seems to be the dominant mechanism exciting the molecular gas (Fig. 18). The ratio \( f_{\text{flu}} \) is low throughout the region, the rotational excitation temperature is consistently very high, and the ortho–para H\(_2\) ratio derived from the \( v = 1 \) lines is close to 3 (Table 3 and Fig. 19), these data all being indicative of shock excitation.
Figure 18. CDR diagrams for six positions across the extensive PN NGC 7048. The positions are labelled in Fig. 1; the spectra themselves are shown in Fig. 13. See Fig. 14 for a description of the symbols used.

Figure 19. Spatial variations for three sources, from left to right: CRL 2688, NGC 6302 and 7048. Rotational temperatures (second panel in each figure) are derived from the 1–0 S(3)/S(1) (solid line) and 1–0 S(2)/S(0) (dashed line) ratios. ν = 1 ortho–para ratios (third panels) are derived from the combinations 1–0 S(0), S(1) and S(2) (solid line) and the 1–0 S(1), S(2) and S(3) (dashed lines) lines. The ortho–para ratio for the fluorescent component, corresponding to the values in the CDR panels, is shown by the dot-dashed line. The other parameters are described in the text.

To summarize then, we find that shock excitation may contribute significantly in all phases of PPN and PN evolution, even in high-ionization PN such as NGC 6302 and 6537. Our most complete data sets (see Figs 14 and 18) suggest that shocks dominate in the early PPN stages (CRL 2688) and also when the PN is fully evolved (NGC 7048). However, a fluorescent component is also required to explain the higher-energy level populations, particularly in the intermediate objects (i.e. in the ‘young’ PN) and predominantly toward the core regions in these sources (see again Fig. 19).

Note, however, that in two PPN – potentially two of the very youngest post-AGB sources in our sample (IRAS 20000+3239 and 22272+5435) – H2 emission was not detected at all. This could be due to high extinction (toward the inner shocked surface of a compact, and therefore dense, post-AGB envelope) and/or veiling by the strong continuum emission (both sources are bright in the K band; see Table 1). The observations of Weintraub et al. (1998) and García-Hernández et al. (2002) collectively suggest that sources that are G2 or earlier excite H2 into emission. The observations and, notably, non-detections reported here agree with this finding (the central sources in IRAS 20000+3239 and 22272+5435 are G8 and G5, respectively). More sensitive observations of these and other continuum-dominated post-AGB stars are clearly warranted, particularly high-spectral-resolution observations that enhance the line-to-continuum ratio (and therefore the ratio between the line flux and the Poisson noise associated with the continuum).
5 CONCLUSIONS

We present a detailed analysis of the molecular gas excitation across a range of post-AGB, PPN and PN sources, at a number of spatial locations across each source. Regardless of excitation state, H$_2$ line emission is detected in almost all targets, in their bipolar lobes but also in many cases in their equatorial tori. Only in the least evolved post-AGB sources considered, IRAS 20000+3239 and 22272+5435, PPN with G8- and G5-type central sources, do we fail to detect H$_2$ emission. (Note, however, that our sample is biased towards sources that are known to be bright in H$_2$ emission.)

From a detailed analysis of the H$_2$ lines detected, first by simply considering individual line ratios, and then using CDR plots and models that combine shocks with fluorescent excitation, we find that for CRL 2688 and NGC 7048, arguably our least and most evolved targets, respectively, shocks may well dominate the excitation: the H$_2$ line ratios in Table 3 are consistently high across these two regions.

A fluorescent component is needed in all other cases, however, to explain the elevated populations of the higher-energy vibrational states. Fluorescence is probably the major excitation mechanism at intermediate evolutionary stages, particularly in the central core regions.

REFERENCES


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