

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

Christopher J. Davis,^{1*} Michael D. Smith,² Luke Stern,^{1,3} Thomas H. Kerr¹
and Jean E. Chiar^{4,5}

¹Joint Astronomy Centre, 660 North A'ohōkū Place, University Park, Hilo, HI 96720, USA

²Armagh Observatory, College Hill, Armagh BT61 9DG

³Department of Physics, University of Victoria, PO Box 3055 STN CSC, Victoria, BC V8W 3P6, Canada

⁴NASA-Ames Research Centre, Mail Stop 245-3, Moffett Field, CA 94035, USA

⁵SETI Institute, Mountain View, CA 94043, USA

Accepted 2003 May 19. Received 2003 May 2; in original form 2003 March 11

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. Balic 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

*E-mail: c.davis@jach.hawaii.edu

Table 1. Observing log.

Target	RA ¹ (2000.0)	Dec ¹ (2000.0)	Date ²	PA ³
NGC 6302	17 13 44.2	−37 06 06	990718	88°
IRAS 17150+3224	17 18 19.8	−32 27 21	990718	125°
IRAS 17441+2411	17 47 13.5	−24 12 51	990718	17°
Hb 5	17 47 56.2	−29 59 39	990717	76°
NGC 6445	17 49 15.2	−20 00 36	000630	136°
NGC 6537	18 05 13.2	−19 50 34	000630	31°
IRAS 18062+2410	18 08 20.1	24 10 43	000630	90°
M 1-92	19 36 18.9	29 32 51	990717	133°
IRAS 20000+3239	20 01 59.5	32 47 32	990717	90°
NGC 6886	20 12 42.9	19 59 21	990718	54°
CRL 2688 (disc)	21 02 18.7	36 41 36	990717	110°
CRL 2688 (jet)	21 02 18.7	36 41 38	990717	15°
NGC 7048	21 14 14.8	46 17 30	990718	100°
IRAS 21282+5050	21 29 58.5	51 04 00	000630	90°
IRAS 22272+5435	22 29 10.3	54 51 06	990717	90°

¹Position of slit on each target (this is not necessarily the geometric 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).

²UT date observed (year/month/day).

³Position angle, measured east of north.

ions as well as rovibrationally excited molecules such as CO and H₂. 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. H₂ 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 6537) and the rapidly evolving post-AGB/young-PN IRAS 18062+2410. Although all of our PN targets were known to be bright in H₂ 2.122- μ m 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 H₂ 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 PPN (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 H₂ lines at $\sim 2 \mu$ m are often thought to be produced in a dense PDR, where thermal emission derives from warm (~ 1000 K), dense gas that is heated by grain photoelectric heating and by far ultraviolet (FUV) pumping of H₂. As the source ages and expands, however, the molecular gas density drops and only then can the lower-energy H₂ states be populated by non-thermal excitation (fluorescence), and then only for low-mass central stars. However, *shocked* H₂ 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 ($> 10^{-5} M_{\odot} \text{ yr}^{-1}$; Natta & Hollenbach 1998). Notably, H₂ 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 H₂-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 H₂ ortho–para ratio for the fluoresced gas. We also search for a correlation between H₂ 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–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 by 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 continua 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 2. Target background information.

Target	Central star	V^1 (mag)	Angular ² Size (arcsec)	H ₂ detected?	$I_{S(1)}^3$ ($\times 10^{-18}$ W m^{-2} arcsec $^{-2}$)	Classical ⁴ description	Ref ⁵
NGC 6302	WD+G2	7.1	~ 400 arcsec	yes	10	Extended, high-excitation, bipolar PN	a, e, l, s
IRAS 17150–3224	G2 I	15.1	~ 8 arcsec	yes	–	Bipolar PPN (obscured source)*	b, n, o
IRAS 17441–2411	$\sim G0$	16.4	~ 4 arcsec	yes ⁶	–	Bipolar PPN (obscured source)*	c, n, o
Hb 5	WD?	10.6	~ 60 arcsec	yes	13	Extended, bipolar PN	d, e
NGC 6445	WD?	–	~ 200 arcsec	yes	10	Extended, bipolar PN	a, e, l, t
NGC 6537	WD	12.3	~ 240 arcsec	yes	8	Extended, high-excitation, bipolar PN	d, e, l, s
IRAS 18062+2410	B1 II	11.1	–	yes	–	Compact, young PN	f
M 1-92	B0.5 V	10.4	~ 12 arcsec	yes	20	Bipolar PPN (partly obscured source)*	g, h, u
IRAS 20000+3239	G8 Ia	12.7	< 2 arcsec	no	–	Round PPN (obscured source)	i, p
NGC 6886	WD	12.9	~ 6 arcsec	yes	4	Compact, high-excitation young PN	j
CRL 2688 (disc)	F5 I	9.0	~ 15 arcsec	yes	5 ⁷	Bipolar PPN (obscured source)*	k, r
CRL 2688 (jet)	F5 I	9.0	~ 20 arcsec	yes	5 ⁷	“ “ “	k, r
NGC 7048	WD?	–	~ 60 arcsec	yes	4	Extended, elliptical PN	a, l
IRAS 21282+5050	WC11	14.3	< 7 arcsec	yes	–	Elliptical, young PN (obscured source)	m, q
IRAS 22272+5435	G5 Ia	8.1	< 4 arcsec	no	–	Elliptical PPN (bright source)*	i, o

¹Approximate V -band magnitudes of the source and/or central nebula taken from the *HST* guide star catalogue, except for the three faintest *IRAS* sources, where values were taken from Ueta et al. (2000) or Kwok et al. (1993). Magnitudes are not given for the diffuse, extended PN, where the central source magnitude is < 19 (for the other PN, the values correspond to the bright core regions only).

²Approximate diameter of line-emission regions, based on optical and/or near-IR morphology (fainter, extended halos may also be present).

³Approximate peak surface brightness in H₂ 1–0 S(1) emission, measured from the images in Fig. 1 (accurate to within 30 per cent).

⁴Description of source morphology [compact (unresolved), round, ring, elliptical or bipolar] and evolutionary state (PPN, young PN or PN): PPN are considered to have effective temperatures between those of AGB stars and CSPNs, detached dust envelopes after AGB mass loss has ended (signified by double-peaked SEDs) and essentially ‘neutral’ nebulae. PN by comparison are signified by strong He I and H I recombination lines, while ‘young PN’ are considered to have the properties of PPN though with weak recombination lines and/or radio continuum, signifying that ionization has recently begun. Obscured source indicates lobes orientated in the plane of the sky; bright source suggests a ‘face-on’ orientation.

⁵References to source size and morphology, CSPN spectral type, etc.: (a) Zhang & Kwok (1998), (b) Kwok et al. (1998), (c) Su et al. (1998), (d) Corradi & Schwartz (1993), (e) Corradi & Schwartz (1995), (f) Arkhipova et al. (1999), (g) Herbig (1975), (h) Bujarrabal et al. (1998a), (i) Hrivnak et al. (1994), (j) Hyung et al. (1995) (k) Crampton, Cowley & Humphreys (1975), (l) Kastner et al. (1996), (m) Kwok et al. (1993), (n) Hu et al. (1993), (o) Ueta et al. (2000), (p) Hrivnak et al. (1999), (q) Meixner et al. (1997), (r) Sahai et al. (1998b), (s) Rowlands et al. (1994), (t) van Hoof et al. (2000), (u) Bujarrabal et al. (1998a).

⁶H₂ line emission detected toward IRAS 17441–2411 by Weintraub et al. (1998).

⁷From Skinner et al. (1997).

*The morphologies of these targets are confirmed with published *HST* imaging.

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 observed just prior to the target itself (H I emission or absorption lines, if present in the standard star spectrum, were removed first). Note, however, that shortward of 2.10 μ m and longward of 2.35 μ m

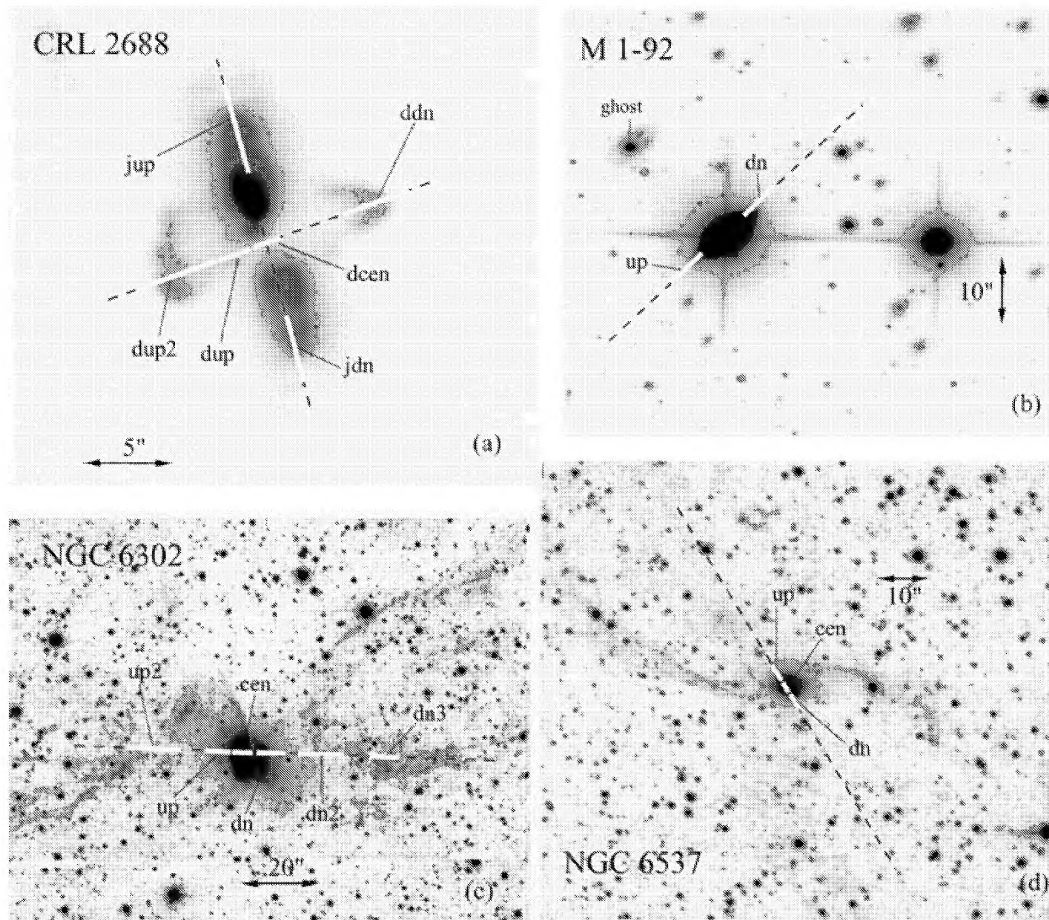


Figure 1. Narrow-band 2.122- μm images of two of the PPN (CRL 2688 and M 1-92) and six of the PN. The dashed lines indicate the position and angles of the slits used in each case; the areas along each slit over which spectra were extracted and added are also indicated with white blocks.

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 H₁ 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 $0.091 \text{ arcsec pixel}^{-1}$, giving a field of view of 92 arcsec. Five-point mosaics were obtained of each target, through 2.122 μm ($\Delta\lambda = 0.02 \mu\text{m}$) H₂ 1–0 S(1) and 2.270 μm ($\Delta\lambda = 0.02 \mu\text{m}$) 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.

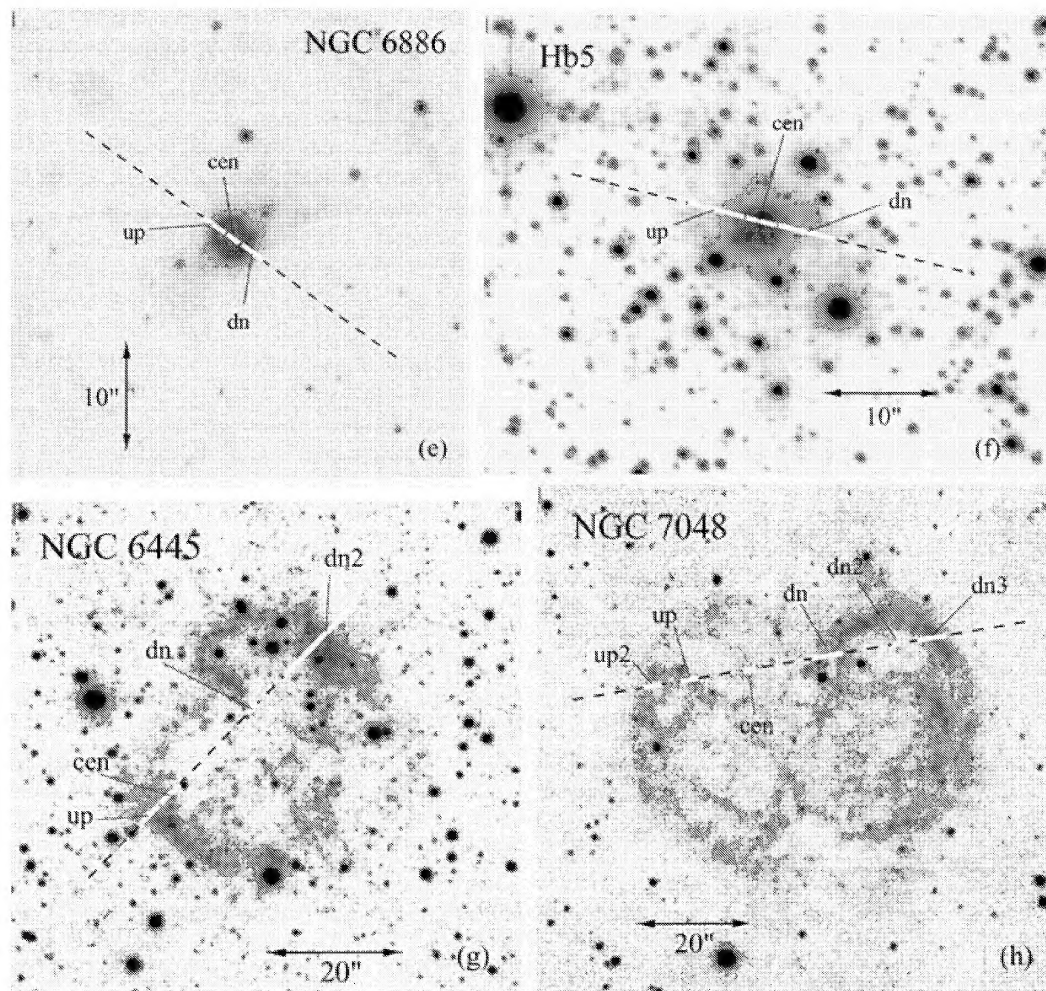


Figure 1 – continued

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 ($PA \sim 19^\circ$) and lie between the two optical, search-light beams described above (Sahai

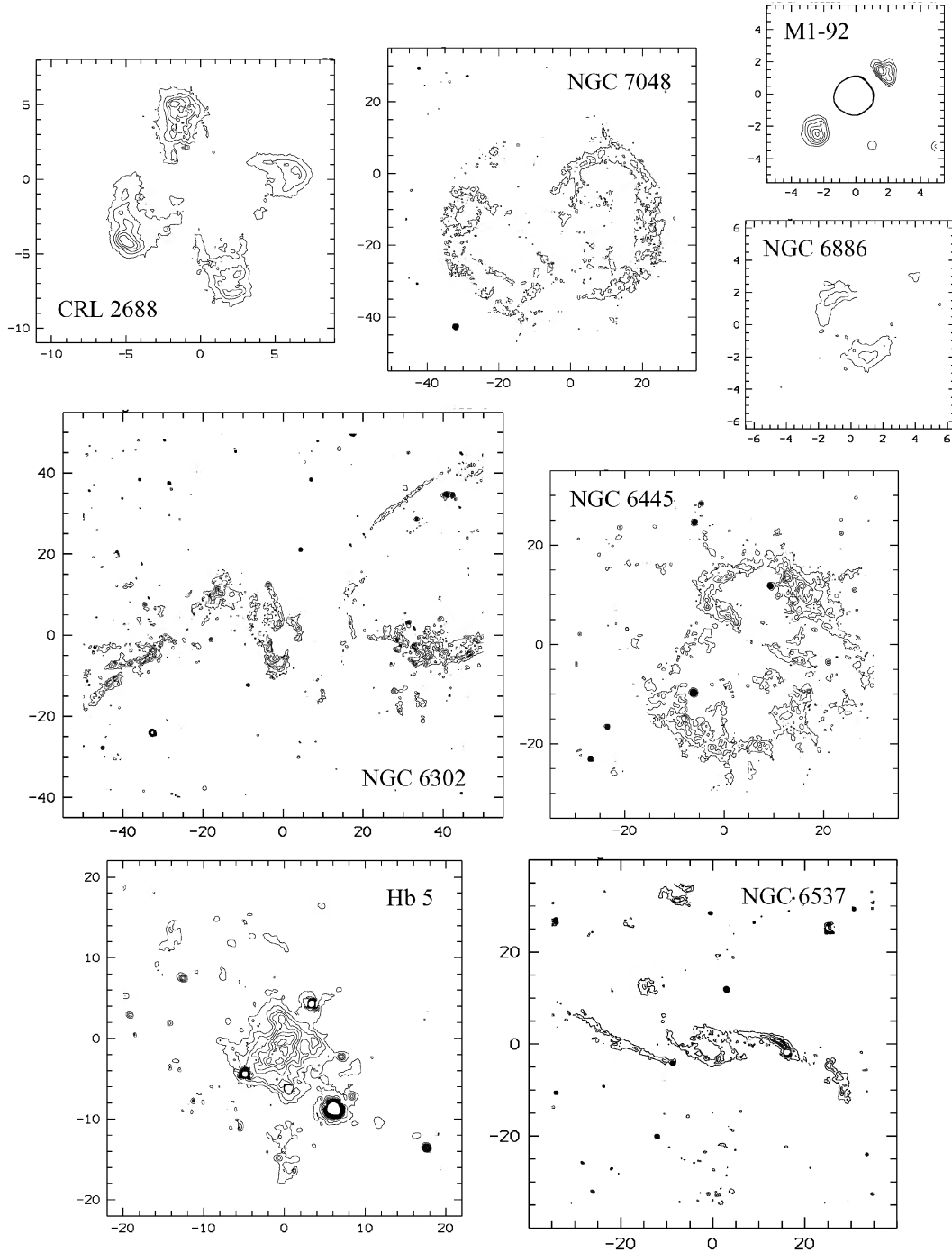


Figure 2. Contour plots showing the continuum-subtracted 2.12- μm images of the target (P)PN. The contours in each plot start at $1.5 \times 10^{-18} \text{ W m}^{-2} \text{ arcsec}^{-2}$ and increase in linear intervals of $1.5 \times 10^{-18} \text{ W m}^{-2} \text{ arcsec}^{-2}$ except for NGC 7048 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 H₂ 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 H₂ 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. H₂ emission lines are detected at all locations. Br γ 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 ($\sim 20\,000$ 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 $200\text{--}300\text{ km s}^{-1}$ (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 $2\text{--}3$ arcsec.

In Fig. 1(b) we present our narrow-band image of M 1-92. At $2\text{ }\mu\text{m}$ 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 H₂ emission, one in each lobe; our continuum-subtracted image in Fig. 2 shows the same H₂ features along the polar jet axis. The H₂ knot in the NW lobe is triangular is

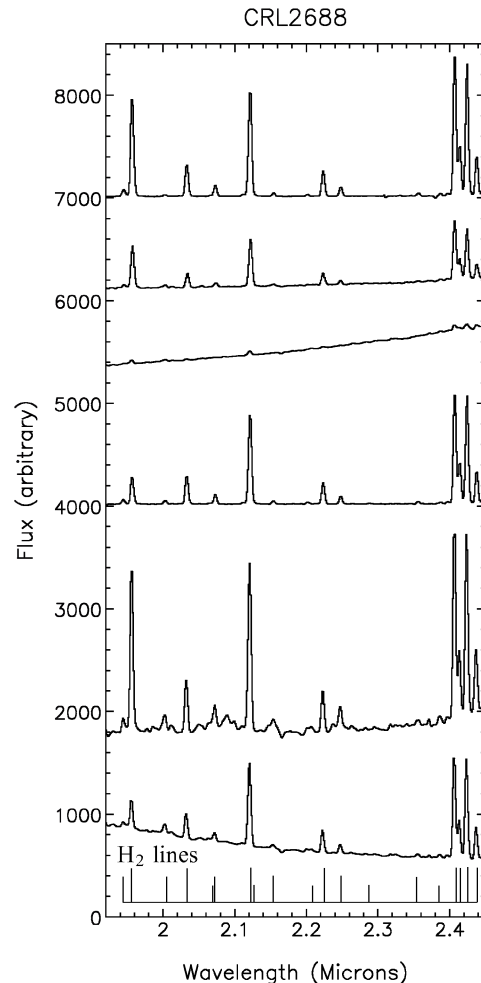


Figure 3. Spectra along two perpendicular axes (slit positions) were observed in CRL 2688; through the ‘disc’ and through the ‘jet’. From top to bottom, the spectra represent the regions labelled dup2, dup, dcen, ddn (through the disc) and jup, jdn (along the jet) in Fig. 1(a). The positions of the most prominent H₂ lines are marked (long tick, $v = 1\text{--}0$ transitions; medium tick, $v = 2\text{--}1$ transitions; small tick, $v = 3\text{--}2$ transitions).

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 γ and the CO bandheads in emission. With our new spectra we can confirm their presence in both bipolar lobes. We also detect H₂ emission from both lobes (Hora et al. report a tentative detection in the NW lobe) though we do not detect H₂ toward the core region. The H₂/Br γ 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

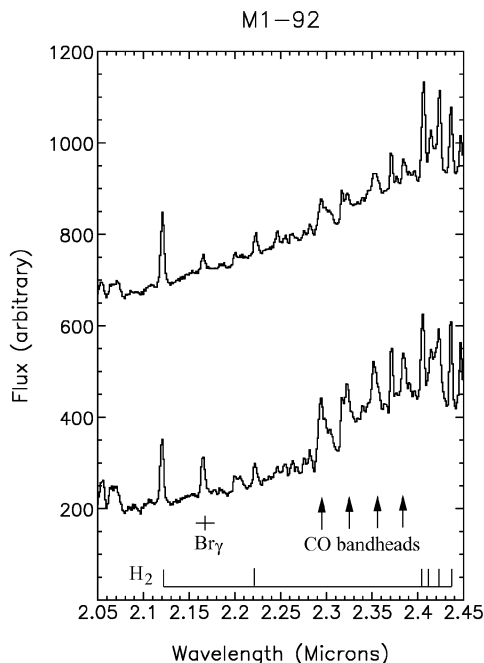


Figure 4. H_2 was observed in the two lobes of the PPN M 1-92; no bright H_2 was detected toward the central region (although $Br\gamma$ and CO bandheads were detected in all three regions). The spectra presented are from the two bipolar lobes; the regions are labelled up (top spectrum) and dn (bottom 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 17441–2411, 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

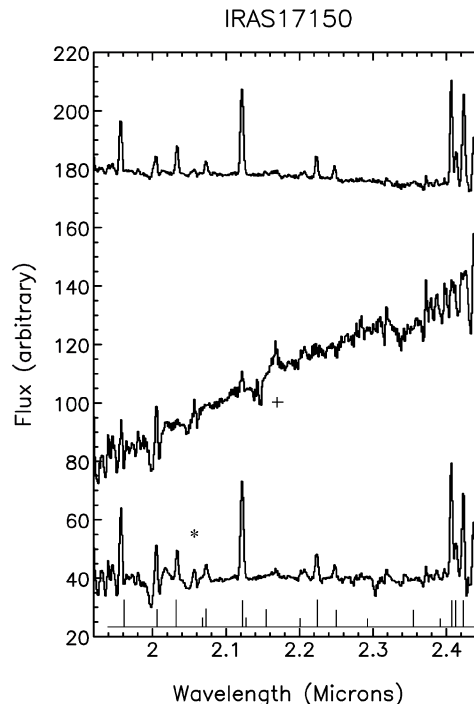


Figure 5. H_2 was observed in the two lobes of the compact PPN IRAS 17150–3224. From top-to-bottom, spectra from regions to the SW, centre and NE of the target are presented; these correspond to up, cen, and dn in the CDR plots (Fig. 15). The SW (up) and NE (dn) spectra cover 3-arcsec long sections of the slit; both regions are offset by 3 arcsec from the central source. The cen spectrum shows emission from the central source itself. (Unfortunately, no images of this PPN were secured, though see Kwok et al. 1998 for high-resolution optical images.) Locations of H_2 lines are marked with ticks (not all lines detected, see Fig. 3). $Br\gamma$ is marked with a cross and He I at 2.058 μm with a star.

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 17441–2411 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 17441–2411 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

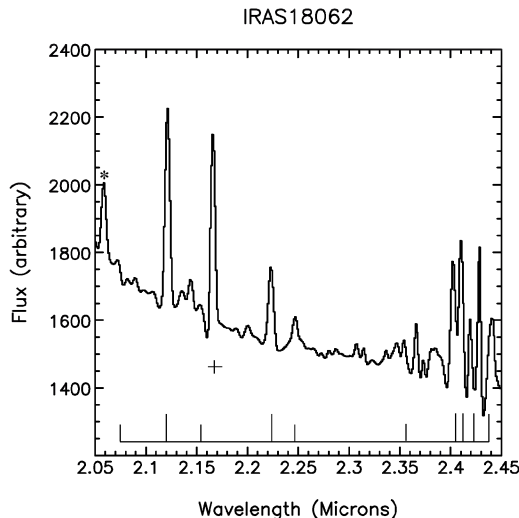


Figure 6. H_2 (and $Br\gamma$) was observed toward the compact, young PN IRAS 18062+2410, though the source was (spatially) unresolved. $Br\gamma$ is marked with a cross, $He\ I$ is marked with a star, and $H_2\ v = 1-0$ and $v = 2-1$ transitions are marked with ticks.

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 $Br\gamma$ 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 (Likkell 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 $Br\gamma$ 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

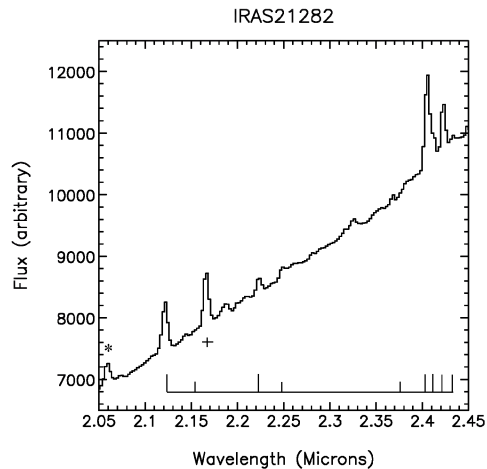


Figure 7. The PPN IRAS 21282+5050 was unresolved in our CGS4 data, so only one spectrum is presented. However, H_2 (and $Br\gamma$) are clearly observed towards this source. $Br\gamma$ is marked with a cross, $He\ I$ is marked with a star, and $H_2\ v = 1-0$ and $v = 2-1$ transitions are marked with ticks.

& 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 $Br\gamma$ and CO bandheads (longward of 2.25 μm) 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 $[\text{Ne}\ \text{v}]$ and $[\text{Si}\ \text{vi}]$ have been observed, ions that require photons with energies ~ 100 – $200\ \text{eV}$ to form. Both objects therefore

probably have massive progenitors, stars that just avoid the supernova stage. In optical images (Corradi & Schwartz 1995; Zhang & Kwok 1998) and infrared images (Figs 1c, d and 2) NGC 6302 and 6537 comprise a bright, compact core with faint lobes of line emission and scattered light extending roughly E–W (NGC 6302) and NE–SW (NGC 6537). Overall, both objects have a bipolar or ‘butterfly’ morphology and are thought to be associated with very hot (250 000 K) white dwarf stars (Casassus et al. 2000). NGC 6302 is also thought to be associated with a binary central star system, comprising a white dwarf and a G-type companion (Feibelman 2001). The CSPNs in both objects are, however, obscured by a dense dust envelope. The high excitation lines observed in NGC 6302 and 6537 may be due to some 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 & Mampasso 1995). Both nebulae also exhibit strong polycyclic aromatic hydrocarbon (PAH) emission (Roche et al. 1996).

Kastner et al. (1996) imaged both nebulae in H₂ emission. Like them, we detect H₂ 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 H₂ emission in the core appears to be confined to an equatorial ring (diameter ~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 H₂ 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 γ emission dominates in the core regions in both sources, as one would expect for these high-excitation nebulae. In NGC 6302 the H₂ 1–0 S(1) emission line begins to dominate in the limb-brightened lobes.

We also detect Br δ at 1.944 μ m, He I (at 2.058 and 2.112 μ m), He II (2.189 μ m) and [Fe III] (2.347 μ 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 & Czyzak 1979; Hyung, Keyes & Aller 1995). Weinberger (1989) and Taylor, Gussie & 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 & 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

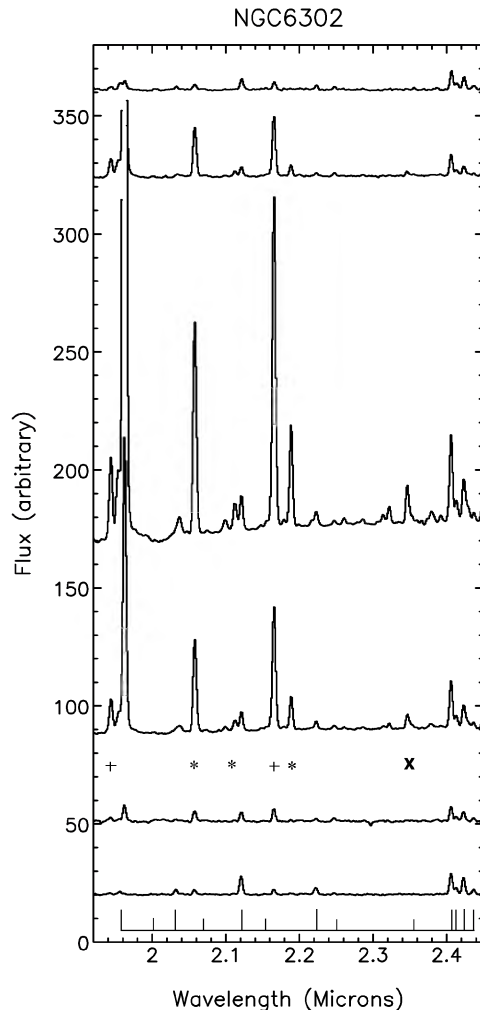


Figure 8. Spectra were observed at six locations across the extended, bipolar planetary nebula NGC 6302; spectra from the bright core and more diffuse lobes are plotted. From top-to-bottom, the spectra represent the regions labelled up2, up, cen, dn, dn2, dn3 in Fig. 1(c). H I bracket lines are marked with crosses; He I (2.058 and 2.122 μ m) and He II (2.189 μ m) lines are marked with stars; [Fe III] (2.347 μ m) is marked with an ‘x’; H₂ lines are marked with ticks.

images we only detect emission from a compact nebula. In Fig. 1(c) 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 H₂ 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 & 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 & Schwartz 1993; Pishmish, Manteiga & 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 & Schwartz 1993), though Hb 5

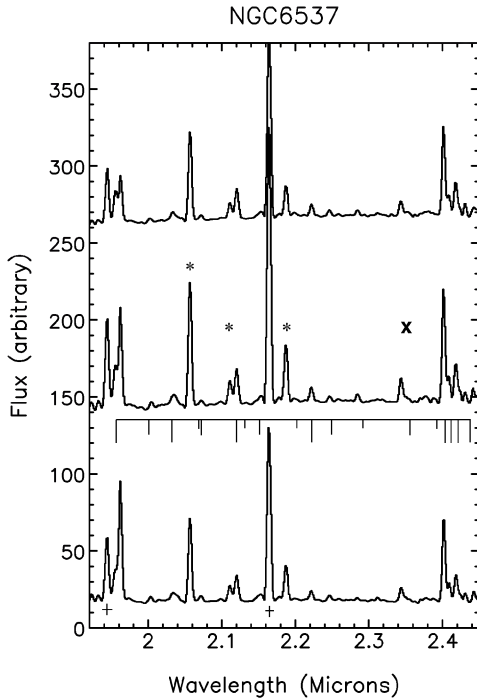


Figure 9. Spectra were extracted from three central regions in the PN NGC 6537; from top-to-bottom, the spectra are from the up, cen and dn regions labelled in Fig. 1(d). See Fig. 8 for a description of line identifications.

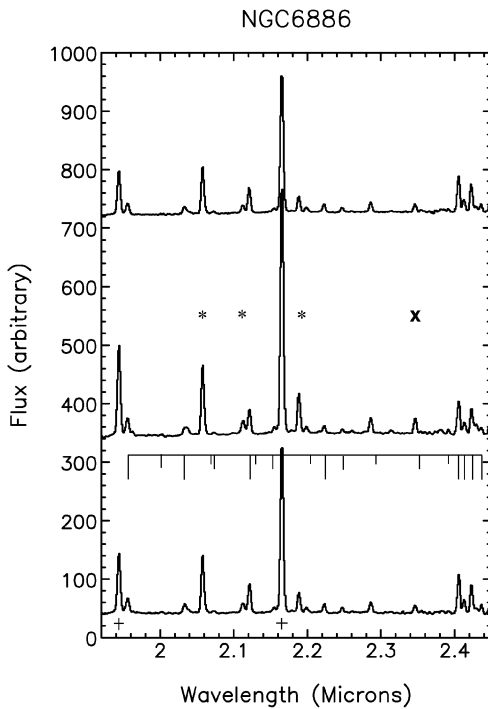


Figure 10. H_2 was only observed in the central core in the PN NGC 6886, though the emission is slightly extended, so three spectra are presented – from top-to-bottom the spectra are from the up, cen and dn areas illustrated in Fig. 1(e). See Fig. 8 for a description of line identifications.

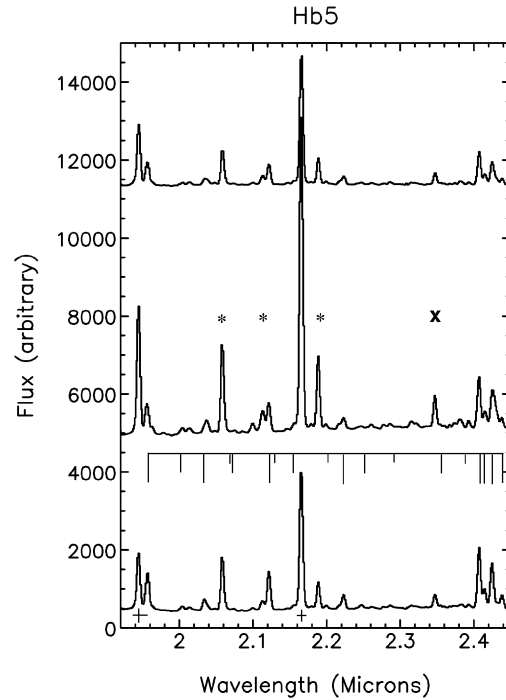


Figure 11. H_2 emission was only detected toward the bright core region of the PN Hb 5; nevertheless, spectra at three locations in this central region are presented. From top-to-bottom the spectra represent areas up, cen, dn (as labelled in Fig. 1f). See Fig. 8 for a description of line identifications.

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 δ at 1.944 μm is also detected in NGC 6886 and Hb 5; the Br γ /Br δ 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 γ /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, ~ 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

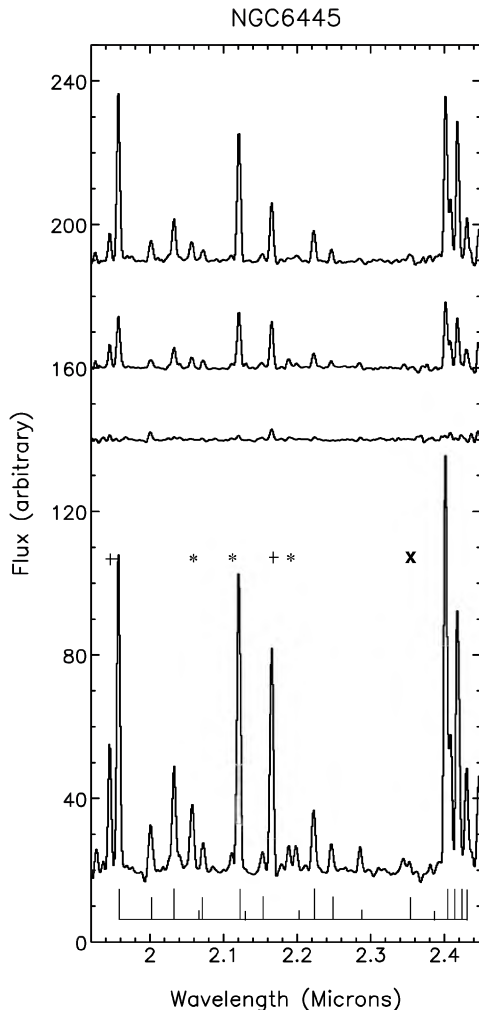


Figure 12. Four spectra were extracted from the one slit observed across the diameter of the ring-shaped PN NGC 6445. The strongest line emission derives from the limb-brightened edges of this PN. From top-to-bottom, the spectra are from the regions labelled up, cen (along the SE edge of PN), dn (near the centre of the ring) and dn2 (the extended, NW edge of PN). These regions are illustrated in Fig. 1(g). See Fig. 8 for a description of line identifications.

inner ring (Fig. 2; see also Kastner et al. 1996). Indeed, this ring is morphologically very similar in H₂, H I, [S II] and [O III], and it is thought to represent a region of enhanced density (Cuesta & Phillips 1999). Note that similar molecular rings are evident in NGC 6537 and, probably also NGC 6302 (Fig. 2), albeit on a smaller angular scale.

Four K-band spectra observed across the nebula are shown in Fig. 12. The H I, He I and He II nebula lines mentioned above are evident across the region, as are the H₂ lines. The H₂ 1–0 S(1)/Br γ line ratio increases toward the molecular ring, as one would expect for an ionized bubble bounded by a molecular ring.

3.2.4 NGC 7048

NGC 7048 is an extensive, evolved PN that was shown to be bright in H₂ 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-

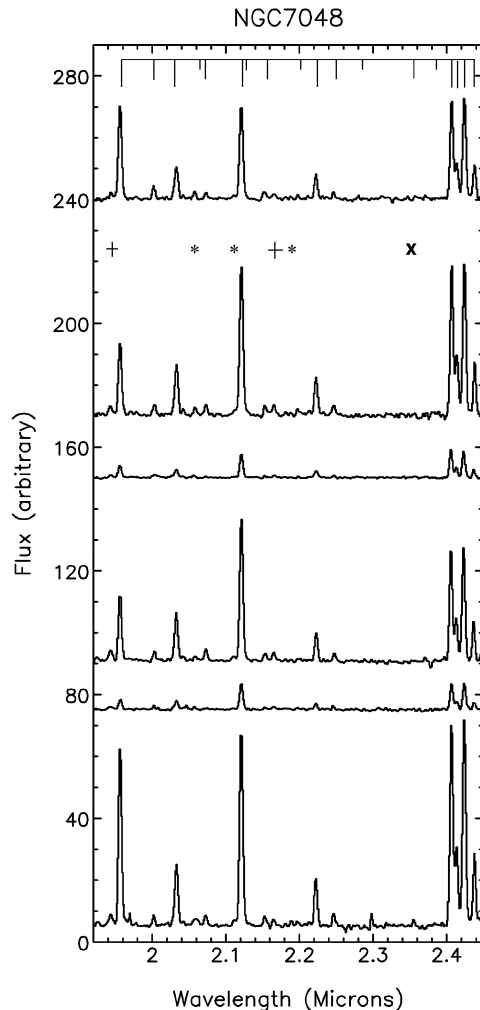


Figure 13. Spectra were observed at six locations across the diameter of the extended PN NGC 7048. From top-to-bottom, the spectra derive from the regions labelled up2, up, cen, dn, dn2, dn3 in Fig. 1(h). See Fig. 8 for a description of line identifications.

IR image (Figs 1h and 2) suggests a possible bipolar or ‘butterfly’ morphology (i.e. a nebula with a waist) with the approximately east–west-orientated lobes of the nebula tilted at $\sim 60^\circ$ to the line of sight (as suggested by comparison with the models of Zhang & Kwok 1998). The H₂ emission seems to delineate a sharp though clumpy boundary between a hot, though relatively diffuse, ionized bubble and the surrounding AGB envelope. The rather low mean electron density and low surface brightness (at optical and infrared wavelengths) of this object suggests that it is quite evolved (Sabbadin, Falomo & Ortolani 1987). Indeed, in our K-band spectra we detect only very weak nebula emission lines (from H I, He I, He II, etc.). The spectra, presented in Fig. 13, are dominated by H₂ emission lines from the molecular boundary evident in the H₂ imaging.

4 ANALYSIS OF THE H₂ DATA

4.1 Line ratios, excitation and the H₂ 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 H₂ 1–0 S(1), 2–1 S(1) and 3–2 S(3) lines (at 2.121, 2.247 and 2.201 μ m), Br γ (at 2.166 μ m) and He I (at 2.058 μ m).

Target ¹	A_K^2	1–0 S(1)/2–1 S(1)	1–0 S(1)/3–2 S(3)	1–0 S(1)/Br γ	1–0 S(1)/He I	ϕ_1^3	ϕ_2^3
<i>PPN (and young PN):</i>							
CRL 2688 (jet)							
- jup	1.8	5.2 ($\pm$ 0.5)	>26	–	>32	3.3	–
- jdn	2.3	8.4 ($\pm$ 1.0)	>45	–	>40	3.2	2.9
CRL 2688 (disc)							
- dup2	2.0	10.1 ($\pm$ 0.4)	58 ($\pm$ 9)	>200	>500	3.2	3.4
- dup	1.7	13.5 ($\pm$ 3.0)	>41	>45	>200	3.1	–
- dcen	0	–	–	–	–	–	–
- ddn	2.1	10.2 ($\pm$ 0.6)	44 ($\pm$ 13)	>400	>400	3.1	3.0
M 1–92							
- up	0	–	–	3.8 ($\pm$ 0.4)	–	–	–
- dn	0	–	–	1.4 ($\pm$ 0.4)	–	–	–
IRAS 17150–3224							
- up	1.7	6.1 ($\pm$ 0.8)	>14	>28	>10	3.0	–
- cen	–	–	–	0.24 ($\pm$ 0.1)	–	–	–
- dn	0.1	6.6 ($\pm$ 1.6)	>10	>17	>5	3.0	–
IRAS 18062+2410							
- cen	0	5.0 ($\pm$ 1.5)	20 ($\pm$ 8)	1.2 ($\pm$ 0.1)	2.0 ($\pm$ 1.0)	2.3	2.4
IRAS 21282+5050							
- cen	2.0	4.2 ($\pm$ 1.5)	>10	0.8 ($\pm$ 0.1)	2.1 ($\pm$ 0.5)	3.0	–
<i>PN:</i>							
NGC 6302							
- up2	2.5	3.5 ($\pm$ 0.9)	–	1.3 ($\pm$ 0.2)	2.5 ($\pm$ 0.4)	2.7	–
- up	0.5	3.2 ($\pm$ 0.7)	7.5 ($\pm$ 2.3)	0.16 ($\pm$ 0.04)	0.20 ($\pm$ 0.01)	2.7	–
- cen	2.4	6.7 ($\pm$ 1.4)	>12	0.10 ($\pm$ 0.01)	0.19 ($\pm$ 0.01)	–	–
- dn	2.0	3.9 ($\pm$ 0.6)	>11.5	0.14 ($\pm$ 0.01)	0.22 ($\pm$ 0.01)	2.0	–
- dn2	2.2	2.1 ($\pm$ 0.8)	>7	0.6 ($\pm$ 0.1)	1.0 ($\pm$ 0.2)	–	–
- dn3	0.9	12.6 ($\pm$ 2.0)	–	3.9 ($\pm$ 0.4)	4.3 ($\pm$ 0.5)	2.4	–
NGC 6537							
- up	3.1	4.2 ($\pm$ 1.8)	–	0.14 ($\pm$ 0.01)	0.38 ($\pm$ 0.02)	2.3	0.6
- cen	2.3	8.4 ($\pm$ 2.5)	>11	0.10 ($\pm$ 0.01)	0.32 ($\pm$ 0.01)	2.3	0.9
- dn	1.9	4.0 ($\pm$ 1.8)	–	0.13 ($\pm$ 0.01)	0.33 ($\pm$ 0.02)	2.1	1.0
NGC 6886							
- up	1.4	6.1 ($\pm$ 0.6)	–	0.17 ($\pm$ 0.01)	0.56 ($\pm$ 0.03)	2.5	1.2
- cen	0	10.5 ($\pm$ 2.0)	–	0.11 ($\pm$ 0.01)	0.38 ($\pm$ 0.03)	2.5	2.7
- dn	0.6	5.8 ($\pm$ 0.5)	–	0.17 ($\pm$ 0.01)	0.50 ($\pm$ 0.03)	2.4	0.6
Hb 5							
- up	0	13.1 ($\pm$ 2.0)	17 ($\pm$ 8)	0.15 ($\pm$ 0.01)	0.56 ($\pm$ 0.01)	1.8	–
- cen	0	2.6 ($\pm$ 1.0)	>5	0.10 ($\pm$ 0.01)	0.36 ($\pm$ 0.01)	2.4	–
- dn	0	12.2 ($\pm$ 2.0)	18 ($\pm$ 6)	0.27 ($\pm$ 0.01)	0.71 ($\pm$ 0.02)	2.1	–
NGC 6445							
- up	1.3	10.2 ($\pm$ 2.0)	24 ($\pm$ 2)	2.0 ($\pm$ 0.1)	7.5 ($\pm$ 1.0)	3.1	1.4
- cen	0.3	8.3 ($\pm$ 3.0)	13 ($\pm$ 6)	1.2 ($\pm$ 0.1)	4.9 ($\pm$ 0.3)	2.8	1.2
- dn	–	–	–	0.37 ($\pm$ 0.02)	–	–	–
- dn2	0	9.8 ($\pm$ 1.0)	13 ($\pm$ 2)	1.4 ($\pm$ 0.1)	4.1 ($\pm$ 0.5)	3.0	1.6
NGC 7048							
- up2	1.7	19.2 ($\pm$ 2.4)	>38	15 ($\pm$ 6)	21 ($\pm$ 9)	2.8	0.8
- up	1.4	12.7 ($\pm$ 2.0)	>21	13 ($\pm$ 3)	30 ($\pm$ 10)	2.9	1.6
- cen	2.2	12.3 ($\pm$ 1.8)	–	10 ($\pm$ 1.8)	12 ($\pm$ 3)	2.2	–
- dn	0.3	20.0 ($\pm$ 2.5)	>44	18 ($\pm$ 3)	37 ($\pm$ 15)	3.3	1.5
- dn2	1.5	10.4 ($\pm$ 1.9)	–	8.7 ($\pm$ 1.8)	19 ($\pm$ 5)	3.1	–
- dn3	1.9	14.5 ($\pm$ 0.8)	>39	26 ($\pm$ 2)	14 ($\pm$ 2)	3.0	1.2

¹ See 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 H₂. A zero indicates a line ratio consistent (to within the errors) with no reddening.³ The H₂ ortho–para ratio. The $v = 1$ values (ϕ_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 μ m), while the $v = 2$ values (ϕ_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 μ m), 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 $v = 1$, $J = 3$ rovibrational 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 λ_1 and λ_2) are modified by the factor: $10^{0.4A_k[(\lambda/\lambda_1)^{1.7} - (\lambda/\lambda_2)^{1.7}]}$, where $\lambda = 2.2 \mu\text{m}$ and A_k is the extinction at $2.2 \mu\text{m}$. The Q(3) line occurs in a relative poor part of the K -band atmospheric window, however, so A_k 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 10^5 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 10^5 – 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(1)/3–2 S(3) ratio retains a value of approximately 8 in a dense PDR ($n_{\text{H}} = 10^4$ – 10^7 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 ($n_{\text{H}} = 10^4$ – 10^7 cm^{-3} , FUV flux $\geq 10^4 G_0$) 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 γ and H_2 1–0 S(1)/He I 2¹P–2¹S(2.058 μm) 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 γ 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 γ 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 γ 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 γ ratio should correlate with the evolutionary stage and bipolarity of each PN. They suggests 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 γ 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).

Photoionization of atomic helium (by photons with energies $> 24.6 \text{ eV}$), followed by recombination and cascade to the 2^3S triplet state and then electronic collisional de-excitation to the 2^1P singlet level will yield 2.058- μm emission in PN, given sufficiently high densities ($n_{\text{crit}} \sim 4 \times 10^4 \text{ cm}^{-3}$ for the collisional transition between the 2^3S and 2^1P states). Consequently, the H_2 1–0 S(1)/He I 2¹P–2¹S ratio in Table 3 will, like the H_2 1–0 S(1)/Br γ ratio, distinguish high-excitation objects from their lower-excitation, molecular counterparts. Indeed, the H_2 1–0 S(1)/He I 2¹P–2¹S ratio closely follows the H_2 1–0 S(1)/Br γ 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 γ 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, ϕ_1 , 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 ϕ_1 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 $\sim 200 \text{ K}$ 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 (Sternberg & 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 ϕ_1 with source evolution. The highest values (~ 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 ϕ_1 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 ϕ_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 2–1 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)

$$1/\phi_2 = 0.898(L_2/L_3)^{0.448}(L_2/L_1)^{0.552}. \quad (1)$$

[Note that the above equation yields the reciprocal of ϕ_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 ϕ_2 are less certain than the values for ϕ_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 γ 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 ratios and ϕ_1 values consistent with thermal (and possibly shock) excitation, does, however, have low values for ϕ_2 . These represent the first indication we have of non-thermal excitation playing a role in this target.

4.2 The CDR method

A more sophisticated way of analysing the H₂ 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 H₂ 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_{flu} .
- (ii) The shock excitation temperature, T_r .
- (iii) The H₂ ortho–para ratio for the fluoresced 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 $\lambda^{-1.7}$. 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 H₂ 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 $\log(\text{CDR})$ versus T_j largely uninformative. We therefore display a ‘normalized’ column density ratio, $\text{CDR}/\text{CDR}(2000 \text{ K})$, where the constant $\text{CDR}(2000 \text{ K}) = \exp(-T_j + 6953 \text{ K})/2000 \text{ K}$. 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 $\log[\text{CDR}/\text{CDR}(2000 \text{ K})] = 0$ represents 2000 K gas in LTE, a sloping straight line represents LTE gas at a

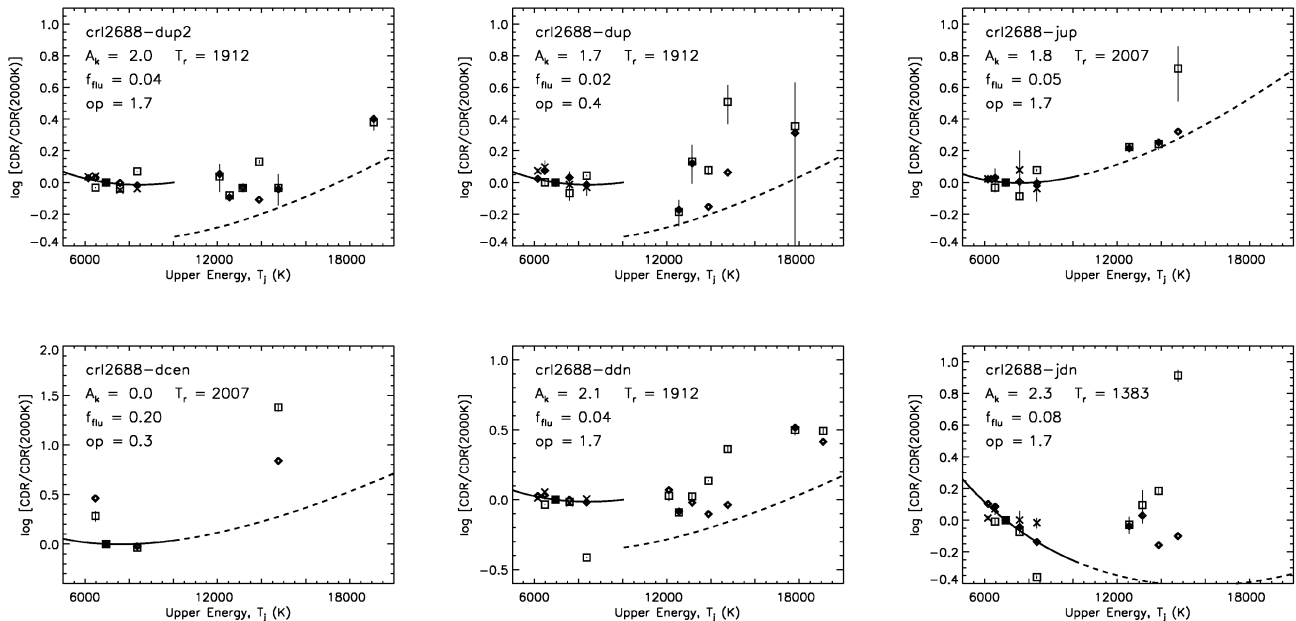


Figure 14. CDR diagrams for the six spectra observed in the PPN CRL 2688. The positions are labelled in Fig. 1; the spectra themselves are shown in Fig. 3. Data points are plotted as boxes (with error bars) except for columns derived from the 1–0 Q-branch lines which are plotted as crosses. The full 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 H₂ ratio, ‘op’, given in each plot (see the text for details). A_k 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.

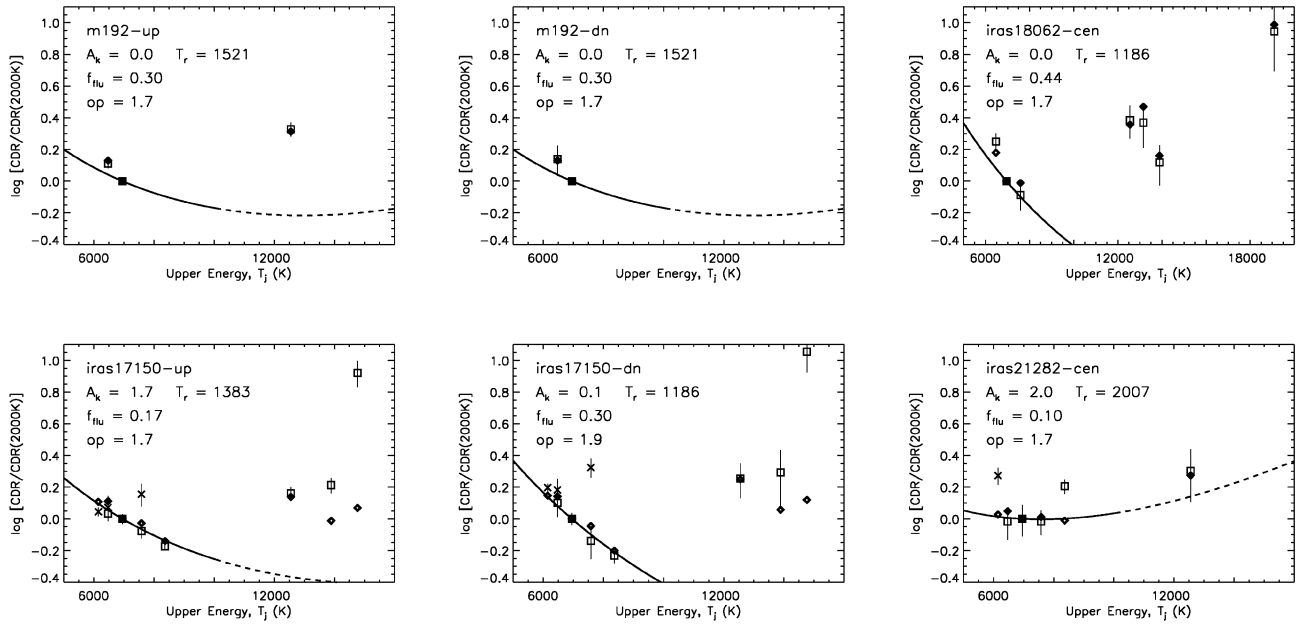


Figure 15. CDR diagrams for the spectra observed in two other PPN, M 1-92 and IRAS 17150–3224, and in two ‘young’ PN, IRAS 18062+2410 and 21282+5050. The separate positions in M 1-92 and IRAS17150–3224 are labelled in Fig. 1; the spectra themselves are shown in Figs 4–7. See Fig. 14 for a description 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.

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 H₂ 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 Dishoeck (1987) (model 14) which

assumes moderate gas densities ($n_H = 3 \times 10^3 \text{ cm}^{-3}$) 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 H₂ 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 H₂ levels predicted by model 14 by a factor of $1.7/\phi$, where a value of ϕ which gives the best fit to the relative rotational distributions is chosen. The value of ϕ used in each case is displayed in each plot (referred to as ‘op’). 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 (ϕ_1) differ markedly; only the (ϕ_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_{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.

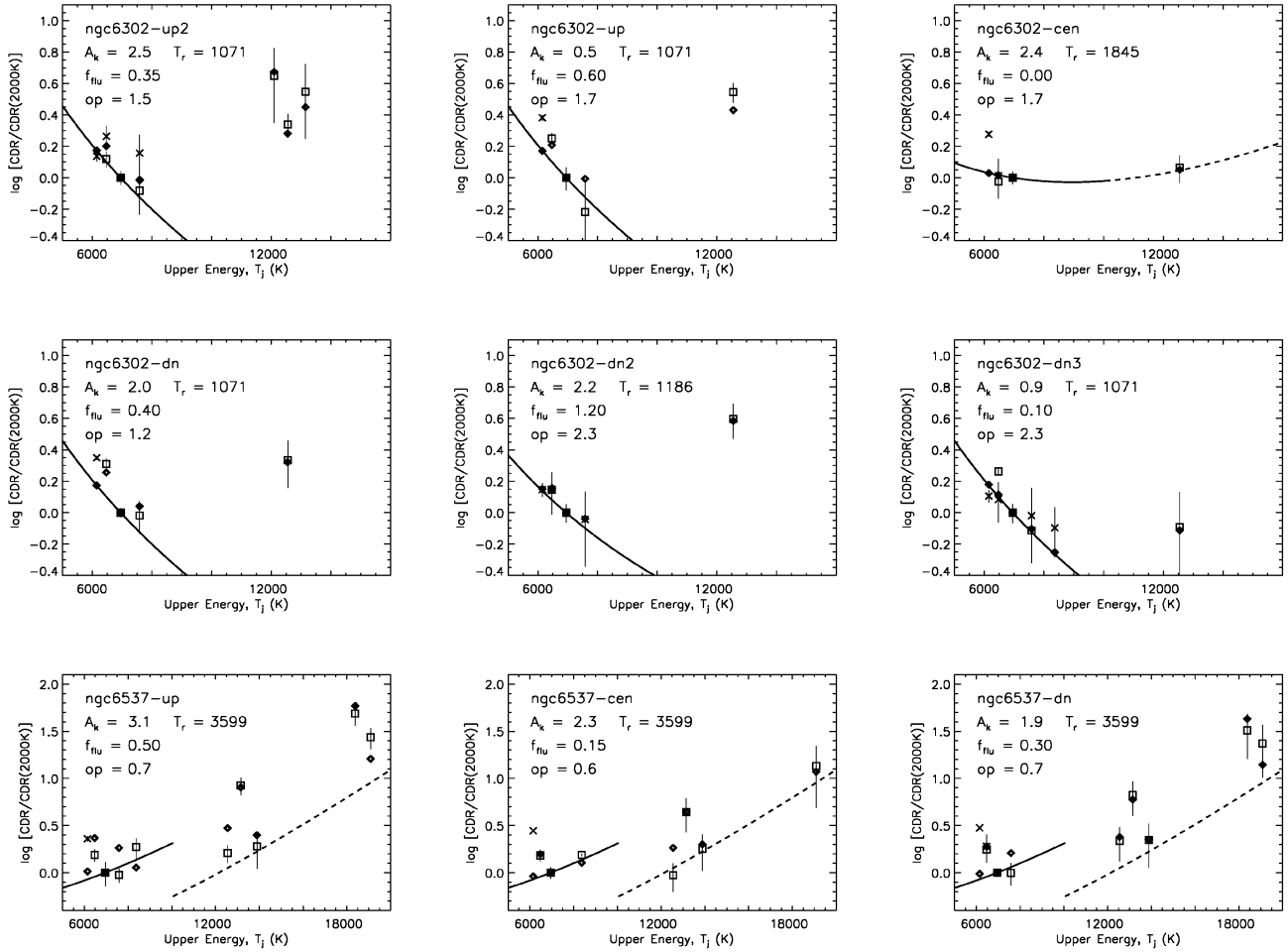


Figure 16. CDR diagrams for six positions and three positions across the high-excitation PN, NGC 6302 and 6537, respectively. The positions are labelled in Fig. 1; the spectra are shown in Figs 8 and 9. See Fig. 14 for a description of the symbols used.

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_{flu} 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 Br γ is detected in both sources (in the latter Br γ 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 Br γ is as bright as the H₂ 1–0 S(1) line. In IRAS 18062+2410 a number

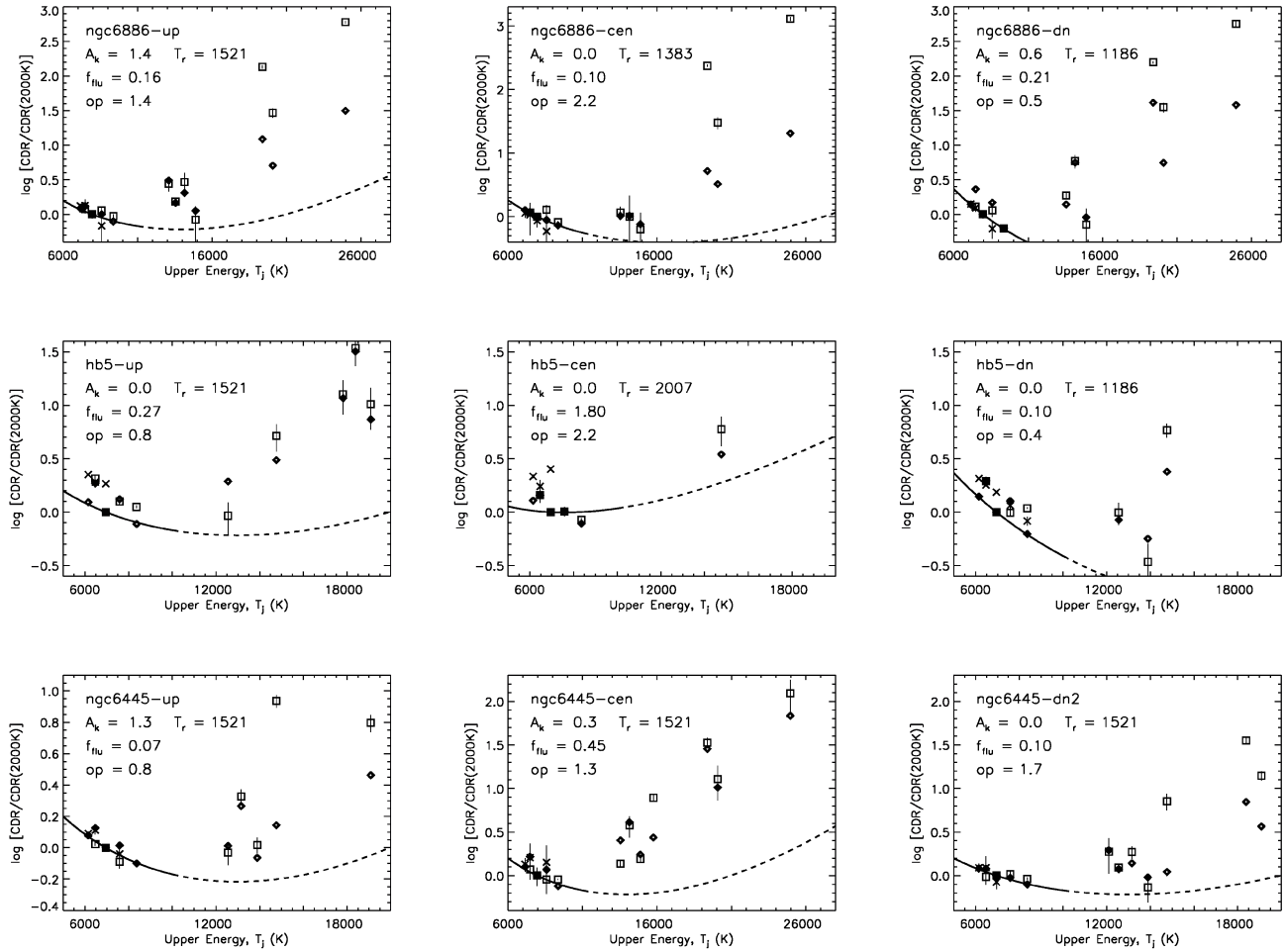


Figure 17. CDR diagrams for three positions across each of the PN; NGC 6886, Hb 5 and NGC 6445. The positions are labelled in Fig. 1; the spectra are shown in Figs 10–12. See Fig. 14 for a description of the symbols used.

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_{flu} is still marginally higher in these targets than in the PPN. In NGC

6302 f_{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 III] 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 ϕ_1 and particularly ϕ_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_{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.

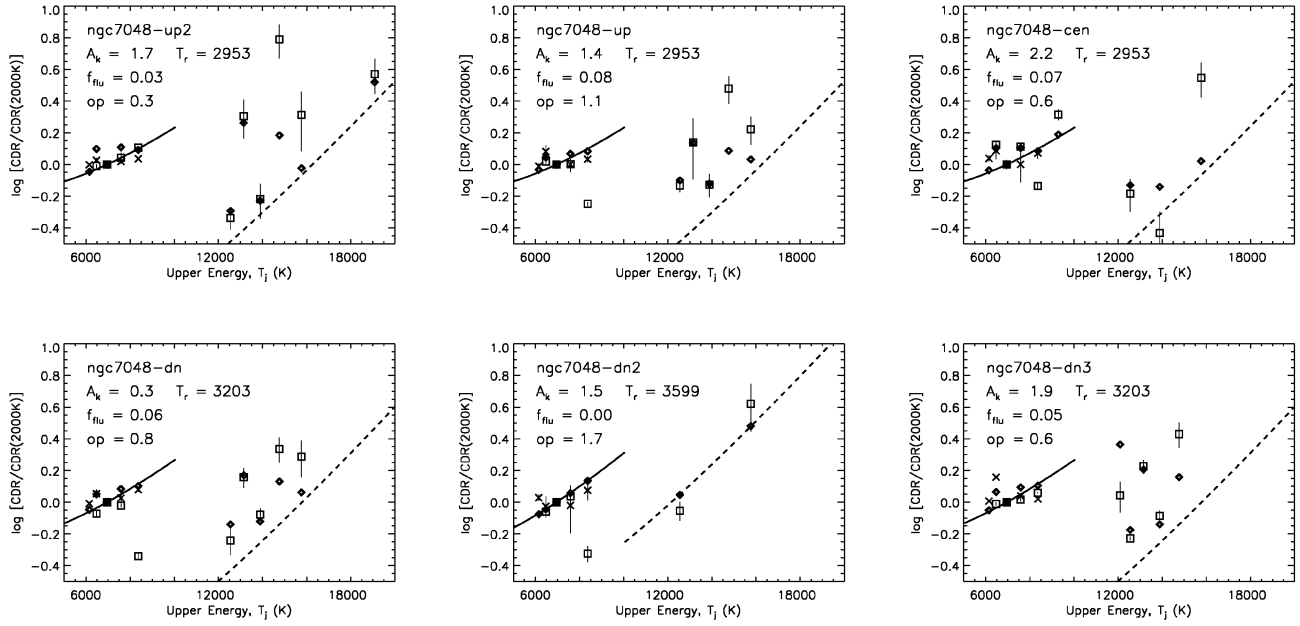


Figure 18. CDR diagrams for six positions across the extensive PN NGC 7048. The positions are labelled in Fig. 1; the spectra themselves are shown in Fig. 13. See Fig. 14 for a description of the symbols used.

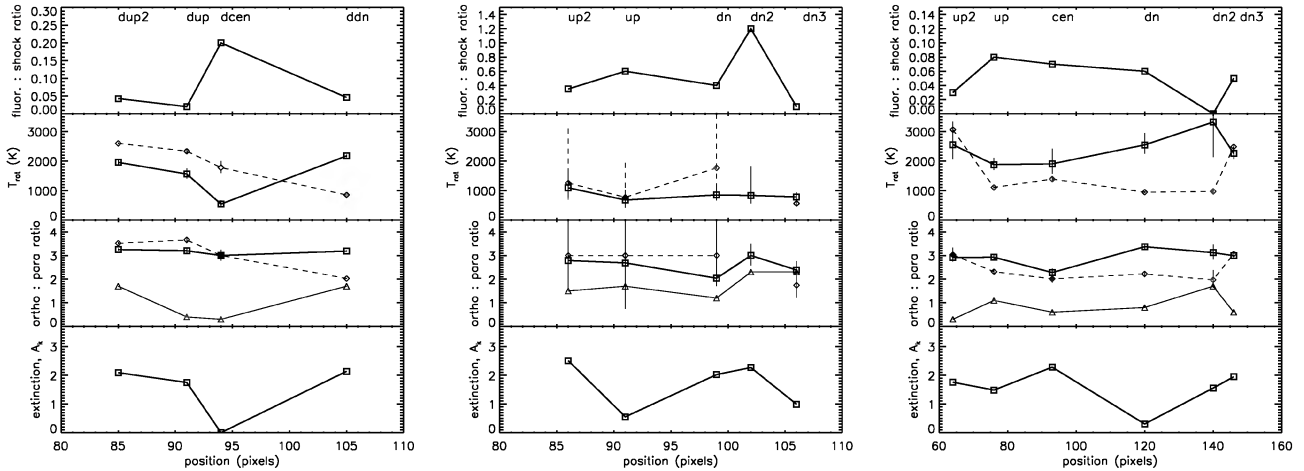


Figure 19. Spatial variations for three sources, from left to right: CRL 2688, NGC 6302 and 7048. Rotational temperatures (second panel in each figure) are derived from the 1–0 S(3)/S(1) (solid line) and 1–0 S(2)/S(0) (dashed line) ratios. $v = 1$ ortho–para ratios (third panels) are derived from the 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) – H_2 emission was not detected at all. This could be due to high extinction (toward the inner shocked sur-

face of a compact, and therefore dense, post-AGB envelope) and/or veiling by the strong dust 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 H_2 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 sources, as are the ortho-para H_2 ratios (particularly for the $v = 1$ states); from the CDR modelling the fluorescent contribution to the gas excitation, represented by f_{fluo} , is low, while the rotational temperature of the $v = 1$ states, T_r , is high.

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.

H_2 emission is usually only observed from bipolar PN and PPN, which in turn are thought to be a morphological class associated with high-mass progenitor stars and high mass-loss rates. Given the additional kinematic and morphological evidence for shocks in (P)PN (given in the introduction and in our description of each source), it is perhaps not surprising, then, that the H_2 excitation may be interpreted with a fluorescence *and* shock model, as we have done here, rather than simply a PDR model, where high densities are used to explain the ‘thermalized’ line ratios from the lower energy levels. Additional high-spectral-resolution H_2 observations would, in any case, be useful for further testing the idea that shocks play a major role in molecular gas excitation in (P)PN.

Finally, given that there may be a time in the post-AGB evolution of a star when H_2 emission becomes detectable or ‘switched-on’, then once this has happened the molecular excitation, derived from the many H_2 lines in the near-IR, may be a useful probe of the evolutionary state of a (P)PN.

ACKNOWLEDGMENTS

We thank Tim Carroll and Thor Wold for their assistance at the telescope, and the referee for his/her thorough review of this article. The UKIRT is operated by the Joint Astronomy Centre on behalf of the UK Particle Physics and Astronomy Research Council; some of the data reported here were obtained as part of the UKIRT Service Programme. JEC is supported by the Long Term Space Astrophysics Program of NASA, grant number 399-20-61-02.

REFERENCES

Aller L.H., Czyzak S.J., 1979, *Ap&SS*, 62, 397
 Arkhipova V.P., Ikonnikova N.P., Noskova R.I., Sokol G.V., Esipov V.F., Klochkova V.G., 1999, *Astron. Lett.*, 25, 25
 Balik B., 1987, *AJ*, 94, 671
 Black J.H., van Dishoeck E.F., 1987, *ApJ*, 322, 412
 Blöcker T., 1995, *A&A*, 299, 755

Bujarrabal V., Alcolea J., Sahai R., Zamarrano J., Zijlstra A.A., 1998a, *A&A*, 331, 361
 Bujarrabal V., Alcolea J., Neri R., 1998b, *ApJ*, 504, 915
 Bujarrabal V., Castro-Carrizo A., Alcolea J., Sánchez Contreras C., 2001, *A&A*, 377, 868
 Burton M.G., Haas M.R., 1997, *A&A*, 327, 309
 Burton M.G., Hollenbach D.J., Tielens A.G.G.M., 1990, *ApJ*, 365, 620
 Burton M.G., Hollenbach D.J., Tielens A.G.G.M., 1992, *ApJ*, 399, 563
 Casassus S., Roche P.F., Barlow M.J., 2000, *MNRAS*, 314, 657
 Corradi R.L.M., Schwartz H.E., 1993, *A&A*, 269, 462
 Corradi R.L.M., Schwartz H.E., 1995, *A&A*, 293, 871
 Cox P. et al., 1997, *A&A*, 321, 907
 Cox P., Lucas R., Huggins P.J., Forveille T., Bachiller R., Guilloteau S., Mallard J.P., Omont A., 2000, *A&A*, 353, L25
 Crampton D., Cowley A.P., Humphreys R.M., 1975, *ApJ*, 198, L35
 Cuesta L., Phillips J.P., 1999, *AJ*, 117, 974
 Cuesta L., Phillips J.P., Mampasso A., 1995, *A&A*, 304, 475
 Davis C.J., Smith M.D., Eisloffel J., Davies J.K., 1999, *MNRAS*, 308, 539
 Dinerstein H.L., Lester D.F., Carr J.S., Harvey P.M., 1988, *ApJ*, 327, L27
 Eisloffel J., Smith M.D., Davis C.J., 2000, *A&A*, 359, 1147
 Feibelman W.A., 2001, *ApJ*, 550, 785
 García-Hernández D.A., Manchado A., García-Lario P., Domínguez-Tagle C., Conway G.M., Prada F., 2002, *A&A*, 387, 955
 Graham J.R., Serbyn E., Herbst T.M., Matthews K., Neugebauer G., Soifer B.T., Wilson T.D., Beckwith S., 1993, *AJ*, 105, 250
 Guerrero M.A., Villaver E., Manchado L., García-Lario P., Prada F., 2000, *ApJS*, 127, 125
 Hawarden T.G. et al., 2001, *MNRAS*, 325, 563
 Herbig G.H., 1975, *ApJ*, 200, 1
 Hollenbach D., Natta A., 1995, *ApJ*, 455, 133
 Hora J.L., Latter W.B., 1994, *ApJ*, 437, 281
 Hora J.L., Latter W.B., Deutsch L.K., 1999, *ApJS*, 124, 195
 Hrivnak B.J., Kwok S., Geballe T.R., 1994, *ApJ*, 420, 783
 Hrivnak B.J., Langill P.P., Su K.Y.L., Kwok S., 1999, *ApJ*, 513, 421
 Hu J.Y., Slijkhuys S., Nguyen-Q-Rieu, de Jong T., 1993, *A&A*, 273, 185
 Hyung S., Keyes C.D., Aller L.H., 1995, *MNRAS*, 272, 49
 Kaler J.B., 1986, *ApJ*, 308, 322
 Kastner J.H., Weintraub D.A., Gatley I., Merrill K.M., Probst R.G., 1996, *ApJ*, 462, 777
 Kastner J.H., Weintraub D.A., Gatley I., Henn L., 2001, *ApJ*, 546, 279
 Kwok S., 1993, *ARA&A*, 31, 63
 Kwok S., Hrivnak B.J., Langill P.L., 1993, *ApJ*, 408, 586
 Kwok S., Hrivnak B.J., Geballe T.R., 1995, *ApJ*, 454, 394
 Kwok S., Hrivnak B.J., Zhang C.Y., Langill P.L., 1996, *ApJ*, 472, 287
 Kwok S., Su K.Y.L., Hrivnak B.J., 1998, *ApJ*, 501, L117
 Latter W.B., Hora J.L., Kelly D.M., Deutsch L.K., Maloney P.R., 1993, *AJ*, 106, 260
 Latter W.B., Kelly D.M., Hora J.L., Deutsch L.K., 1995, *ApJS*, 100, 159
 Likkell L., Morris M., Kastner J.H., Forveille T., 1994, *A&A*, 282, 190
 Lumsden S.L., Puxley P.J., Hoare M.G., 2001, *MNRAS*, 328, 419
 Magazzu A., Strazzulla G., 1992, *A&A*, 263, 281
 Meixner M., Skinner C.J., Graham J.R., Keto E., Jernigan J.G., Arens J.F., 1997, *ApJ*, 482, 897
 Menzies J.W., Wolstencroft R.D., 1990, *MNRAS*, 247, 177
 Mountain C.M., Robertson D., Lee T.J., Wade R., 1990, in *Instruments in Astronomy*, v1235, VII, SPIE, Bellingham, p. 25
 Natta A., Hollenbach D., 1998, *A&A*, 337, 517
 Ney E.P., Merrill K.M., Becklin E.E., Neugebauer G., Wynn-Williams C.G., 1975, *ApJ*, 198, L129
 Parthasarathy M., García-Lario P., Sivarani T., Manchado A., Sanz Fernández de Córdoba L., 2000, *A&A*, 357, 241
 Pishmish P., Manteiga M., Recio A.M., 2000, in *Kastner J.H., Soker N., Rappaport S., eds, ASP Conf Ser. Vol. 199, Asymmetrical PN II: from Origins to Microstructures. Astron. Soc. Pac., San Francisco*, p. 397
 Pottasch S.R., Beintema D.A., Domínguez-Rodríguez F.J., Schaeidt S., Valentijn E., Vandenbussche B., 1996, *A&A*, 315, L261
 Pottasch S.R., Beintema D.A., Feibelman W.A., 2000, *A&A*, 363, 767

- Ramsay S.K., Chrysostomou A., Geballe T.R., Brand P.W.J.L., Mountain M., 1993, MNRAS, 263, 695
- Roche P.F., Lucas P.W., Hoare M.G., Aitken D.K., Smith C.H., 1996, MNRAS, 280, 924
- Rowlands N., Houck J.R., Herter T., 1994, ApJ, 427, 867
- Sabbadin F., Falomo R., Ortolani S., 1987, A&AS, 67, 541
- Sahai R. et al., 1998a, ApJ, 493, 301
- Sahai R. et al., 1998b, ApJ, 492, L163
- Shibata K.M., Tamura S., Deguchi S., Hirano N., Kameya O., Kasuga T., 1989, ApJ, 345, L55
- Shupe D.L., Larkin J.E., Knop R.A., Armus L., Matthews K., Stoifer B.T., 1998, ApJ, 498, 267
- Skinner C.J. et al., 1997, A&A, 328, 230
- Smith M.D., 1995, MNRAS, 296, 789
- Smith M.D., Brand P.W.J.L., Moorehouse A., 1991a, MNRAS, 248, 451
- Smith M.D., Brand P.W.J.L., Moorehouse A., 1991b, MNRAS, 248, 730
- Smith M.D., Davis C.J., Lioure A., 1997, A&A, 327, 1206
- Smith M.D., Khanzadyan T., Davis C.J., 2003, MNRAS, 339, 524
- Solf J., 1994, A&A, 282, 567
- Sternberg A., Neufeld D.A., 1999, ApJ, 516, 371
- Su K.Y.L., Volk K., Kwok S., Hrivnak B.J., 1998, ApJ, 508, 744
- Taylor A.R., Gussie G.T., Pottasch S.R., 1990, ApJ, 351, 515
- Thronson H.A., 1982, AJ, 87, 1207
- Trammell S.R., Goodrich R.W., 1996, ApJ, 468, L107
- Ueta T., Meixner M., Bobrowski M., 2000, ApJ, 528, 861
- van Hoof P.A.M., van de Steene G.C., Beintema D.A., Martin P.G., Pottasch S.R., Ferland G.J., 2000, ApJ, 532, 384
- Vicini B., Natta A., Marconi A., Testi L., Hollenbach D., Draine B.T., 1999, AA, 342, 823
- Volk K.M., Kwok S., 1989, ApJ, 342, 345
- Weinberger R., 1989, A&AS, 78, 301
- Weintraub D.A., Huard T., Kastner J.H., Gatley I.A., 1998, ApJ, 509, 728
- Zhang C.Y., Kwok S., 1998, ApJS, 117, 341

This paper has been typeset from a $\text{\TeX}/\text{\LaTeX}$ file prepared by the author.