Molecular Hydrogen *

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Abstract. Observations of H_2 line emission in galactic and extragalactic environments obtained with the Infrared Space Observatory (ISO) are reviewed. The diagnostic capability of H_2 observations is illustrated. We discuss what one has learned about such diverse astrophysical sources as photon-dominated regions, shocks, young stellar objects, planetary nebulae and starburst galaxies from ISO observations of H_2 emission. In this context, we emphasise use of measured H_2 line intensities to infer important physical quantities such as the gas temperature, gas density and radiation field and we discuss the different possible excitation mechanisms of H_2. We also briefly consider future prospects for observation of H_2 from space and from the ground.

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1. Physics of H_2

1.1. Astrophysical importance of H_2

Molecular hydrogen is the most abundant molecule in the Universe and plays a fundamental role in many astrophysical contexts (e.g., Dalgarno, 2000). It is found in all regions where the shielding of the ultra-violet (UV) photons, responsible for its photo-dissociation, is sufficiently large, i.e. where $A_V \gtrsim$ 0.01-0.1 mag. H_2 makes up the bulk of the mass of the dense gas in galaxies and could represent a significant fraction of the total baryonic mass of the Universe. Further on, H_2 plays two main roles that render it key for our understanding of the interstellar medium, in particular of the processes regulating star formation and the evolution of galaxies. Firstly, the formation of H_2 on grains initiates the chemistry of interstellar gas; secondly, H_2 is recognized as a major contributor to the cooling of astrophysical media.

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H_2 has also specific radiative and collision properties that make it a diagnostic probe of unique capability. Many competing mechanisms could contribute to its excitation (see Sect. 1.2) and H_2 can serve as probe of a wide range of physical environments. Thus, as we understand reasonably well its radiative and collisions properties we can construct realistic models of the response of H_2 to its surroundings.

1.2. Excitation and formation of H_2

Containing two identical hydrogen atoms, the hydrogen molecule is highly symmetric. Due to this symmetry, the molecule has no dipole moment and all ro-vibrational transitions within the electronic ground state are quadrupolar with low spontaneous coefficient A values. The molecule exists in two, almost independent states, namely ortho-H_2 (spins of H nuclei parallel) and para-H_2 (spins antiparallel). There are no radiative transitions between ortho- and para- H_2 but ortho-para conversion may occur through proton exchange reactions between H_2 and, for example, H^0 and H^+.

Molecular hydrogen may be excited through several mechanisms: **(1)** In the presence of far-ultraviolet radiation (FUV, $\lambda > 912$ Å), the molecule is radiatively pumped into its electronically excited states. As it decays back into the electronic ground state, it populates the high vibrational levels, and the subsequent cascade to v=0 gives rise to optical and infrared fluorescent emission, and a characteristic distribution of level populations (e.g., Black & van Dishoeck, 1987, Sternberg, 1989). This excitation mechanism is observed in photon-dominated regions (PDRs) where it dominates the excitation of ro-vibrational and high rotational levels. **(2)** If the gas density and temperature are high enough, inelastic collisions can be the dominant excitation mechanism, at least for the lower energy levels (e.g., Le Bourlot et al., 1999). In dense PDRs ($n_H \gtrsim 10^4$ cm^{-3}) and shocks, collisions maintain the lowest pure rotational levels in thermal equilibrium. **(3)** H_2 formation in excited states can also contribute to the excitation of the molecule. **(4)** Finally, in environments such as active galactic nuclei (AGNs) or X-ray emitting young stellar objects where hard X-rays are capable to penetrate deeply into zones opaque to UV photons, X-rays can dominate H_2 excitation (Maloney et al., 1996; Tine et al., 1997).

Except in the early Universe, most H_2 is thought to be produced via surface reactions on interstellar grains (e.g., Gould & Salpeter, 1963, Hollenbach & Salpeter, 1971), since gas-phase reactions are predicted to be too slow. But due to our limited understanding of the relevant properties of interstellar grains (composition, structure and hydrogen coverage) and hence of grain surface reactions, the H_2 formation mechanism is not yet understood. Numerous theoretical and experimental studies have thus been dedicated to a better understanding of the H_2 formation process (Gould & Salpeter, 1963; Hollenbach & Salpeter, 1971; Sandford & Allamandola, 1993; Duley, 1996; Parneix & Brechignac, 1998; Pirronello et al., 1997; Pirronello et al., 1999; Takahashi et al., 1999; Katz et al., 1999; Williams et al., 2000; Sidis et al., 2000; Biham et al., 2001; Joblin et al., 2001; Cazaux & Tielens, 2003; Cazaux & Tielens, 2002). Another approach to this issue is to use observations to provide estimates of the H_2 formation rate in different regions of the ISM in order to see how it depends upon the local physical parameters. Recently, combined ISO (Kessler et al., 1996; Kessler et al., 2003) observations of H_2 line emission and dust emission as well as FUSE observations of UV pumping lines in absorption have highlighted the H_2 formation process (see Sect. 3.1).

2. Observations of H_2

Direct observation of H_2 is difficult. Electronic transitions occur in the ultraviolet, to which the Earth's atmosphere is opaque, and observations can only be made from a space-based platform. Ro-vibrational and rotational transitions are faint because of their quadrupolar origin. In the case of rotational lines which occur in the mid-IR, the Earth's atmosphere is at best only partly transparent. Moreover, most of H_2 may hide in cool, shielded regions (e.g., Combes, 2000) where the excitation is too low to be detected through emission lines and whose extinction is too high to allow the detection of the UV pumping lines.

Space-based missions in the UV (Copernicus, ORPHEUS, FUSE) and the mid-IR (ISO, Spitzer) provide the most stringent tests of our current understanding of H_2 in space.

2.1. UV absorption lines

In the 1970's, the Copernicus satellite observed molecular hydrogen electronic lines in absorption towards nearby early type stars (e.g., Spitzer et al., 1974). This experiment yielded reliable column densities for diffuse clouds ($A_V \leq 1$), the first measurements of the temperature of H_2 in diffuse clouds (~50-100 K) as well as an estimate of the formation rate of H_2 on interstellar dust grains (Jura, 1975). Recently, thanks to the greater sensitivity of FUSE, fainter stars with higher extinctions could be observed allowing the study of translucent clouds (e.g., Rachford et al., 2002). However, such observations are limited by the small number of sufficiently luminous background sources against which H_2 can be detected in absorption. In practice, UV observations only allow the study of molecular gas in the Solar Neighborhood and provide no spatial information on the distribution of H_2.

2.2. Infrared observations

Prior to the advent of ISO, infrared emission of H_2 was observed in the 2 μm ro-vibrational lines (most notably the 1-0 S(1) line at 2.12 μm) towards Galactic shocks and PDRs, planetary nebulae, and in some instances the nuclei of active galaxies (for the first studies see e.g. Shull & Beckwith, 1982, Fischer et al., 1987). However, in PDRs and shocks only a small fraction of the H_2 is vibrationally excited.

The first observations of the $v = 0$ pure rotational lines of H_2 have been done from the ground towards a PDR - the Orion bar - by Parmar et al. (1991). The lowest rotational transitions of H_2 produced by collisions (see Sect. 1.2) provide a thermometer for the bulk of the gas above $\sim$80 K. Also, due to the low A-values of these transitions, optical depth effects are usually unimportant and thus these lines provide accurate measures of the warm ($T \gtrsim 80$ K) gas mass.

With the sensitivity of the ISO instruments (i.e. SWS and CAM) several pure rotational lines of H_2 have been observed in a variety of galactic and extragalactic environments. Moreover for each type of environment, numerous objects with a wide range of physical conditions were observed allowing us to address a number of outstanding questions concerning the physics of H_2. Moreover, the complete ISO wavelength coverage (2-200 μm), which includes many lines due to gas-phase atoms (e.g., C^+, O^0, Si^+, S^0), molecules (e.g., H_2, CO, H_2O, OH and CO_2) and bands of polycyclic aromatic hydrocarbons (PAHs), silicates and ices, allows us to study the links between H_2, the dust and the other gas components. A review on ISO spectroscopic results from molecular clouds to disks by van Dishoeck (2004) illustrates the diagnostic capabilities of the various lines and bands detected by ISO.

This article summarizes the ISO spectroscopic observations of H_2. The bulk of the data comes from the Short Wavelength Spectrometer (SWS, 2-45 μm, de Graauw et al., 1996; ?, ?). Relevant spectra have also been obtained with the Camera-Circular Variable Filter (CAM-CVF, 2.3-16.5 μm, Cesarsky et al., 1996; Blommaert et al., 2003).

3. An overview of ISO observations of H_2 in galactic and extragalactic environments

ISO has observed H_2 emission from sources as diverse as photo-dominated regions (PDRs), shocks associated with outflows or supernovae remnants, circumstellar environment of young stellar objects, planetary nebulae, and external galaxies. Combined to theoretical models of PDRs and shocks these observations have allowed the derivation of important physical quantities in these objects, namely, the hydrogen density n_H, the intensity of the incident far-ultraviolet (FUV, 6< $h\nu$ <13.6 eV) radiation represented by χ [1], the H_2 rotational excitation temperature T_{rot} (a measure of the gas temperature, see below) and the H_2 column density N_{H_2}. In this section, these H_2 observations and the inferred physical quantities are reviewed (see Table 1 for a summary).

3.1. Photon-dominated regions

Photon-dominated regions (PDRs) are one of the most important sources of H_2 emission. PDRs form at the surfaces of molecular clouds where FUV radiation encounters and dissociates the dense molecular gas. They are the transition zone between the dense, cold molecular gas and the tenuous, warm, ionized gas (for a recent review see Hollenbach & Tielens, 1999). The thermal and chemical structure of the PDR is governed by the FUV radiation[2] and depends mainly on two parameters, namely, the incident FUV flux χ and the density n_H.

ISO has observed a series of pure H_2 rotational lines towards a number of PDRs sampling a wide range of excitation conditions: high excitation PDRs with $\chi > 10^3$ such as the Orion Bar (Bertoldi et al., priv. com), NGC 2023 (Moutou et al., 1999; Draine & Bertoldi, 2000a), NGC 7023 (Fuente et al., 1999); moderately excited PDRs with $10^2 < \chi < 10^3$ such as IC 63 (Thi et al., 1999), S 140 (Timmermann et al., 1996) and ρ Oph W (Habart et al., 2003); and low excitation PDRs such as the cool PDR Ced 201 (Kemper et al., 1999) or the S 140 extended region (Li et al., 2002). Detailed studies using ISO observations of both H_2 and dust emission, in conjunction with ground-based NIR imaging, allows us to bring new insights mainly into (i) the temperature and density structure of PDRs, (ii) the dominant heating and cooling processes and (iii) the H_2 formation process.

[1] The scaling factor χ represents the intensity of the FUV field in units of the Draine (1978) average interstellar radiation field.

[2] The FUV radiation field sets the PDR chemical structure by ionizing carbon, silicon, etc.., and by dissociating H_2, CO and most other molecules. It also heats the gas mainly via the photoelectric effect on dust grains.

H_2 as a thermal probe in PDRs. At densities $n_H \gtrsim 10^4$ cm^{-3} of bright PDRs, collisions maintain the lowest rotational levels of H_2 (v=0, $J \lesssim$5) in thermal equilibrium. The population of these levels is therefore a good indicator of the gas temperature. This is reflected in their excitation diagrams (see Fig. 1) where their populations are consistent with the Boltzmann law. We report in Table 1 the excitation temperature of the H_2 pure rotational levels for some PDRs with different excitation conditions. All the derived $T_{\rm rot}$ are found to be similar between 300 and 700 K.

It should be noted that, in spite of their simple appearance, the interpretation of these diagrams has to take of account several factors. First, the gas temperature varies rapidly through the PDR layer from several hundred K at the edge close to the excitation source to less than 30 K when $A_V > 1$. The pure rotational H_2 lines arise primarily in the outer warm layer. Second, the excitation temperature of H_2 pure rotational levels gives in principle an upper limit to the kinetic temperature as UV pumping may contribute to the excitation of H_2 even for low J.

For several PDRs observed by ISO, the H_2 line intensities and the gas temperature are found to be higher than predicted by current models (Bertoldi, 1997; Draine & Bertoldi, 1999b; Thi et al., 1999; Habart et al., 2003; Li et al., 2002). The cause of this discrepancy is either that, in the models, the gas is not hot enough or alternatively that the column density of H_2 is too low in the zones where the gas is warm. Several possible explanations have been proposed. An increase of the grain photoelectric heating rate is one possibility. Draine & Bertoldi (2000a) have in particular shown that increased photoelectric heating rates based on an enhanced dust-to-gas ratio in the PDR due to gas-grain drift can reproduce the H_2 observations in the reflection nebula NGC 2023. Another explanation, namely an increased H_2 formation rate, is dicussed below. Finally, non-equilibrium processes, e.g. propagation of the ionization and photodissociation fronts which will bring fresh H_2 into the zone emitting line radiation, can be invoked but detailed models are needed.

H_2 formation rate. Recently, Habart et al. (2004) combined ISO observations of rotational lines of H_2 towards a sample of PDRs with observations of ro-vibrational lines made with ground–based telescopes in order to constrain the formation rate of H_2 under the physical conditions in the layers responsible for H_2 emission. Using as a diagnostic the 0-0 S(3)/1-0 S(1) line ratio, which strongly depends on the value of the H_2 formation rate R_f, they find that, in regions of moderate excitation

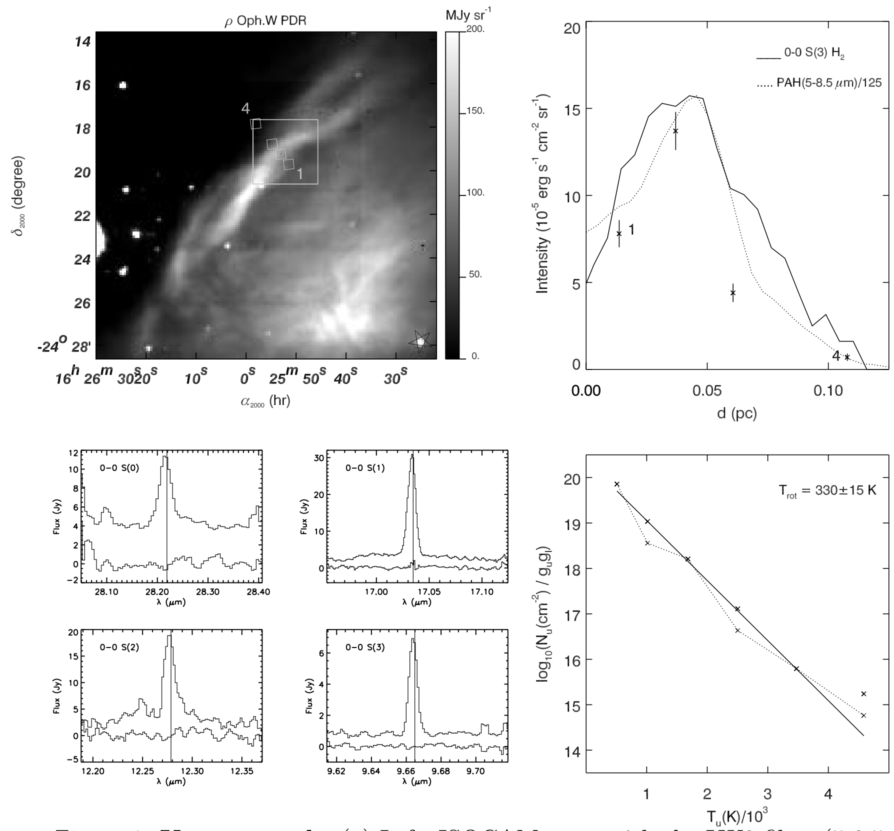

Figure 1. **Upper panels.** (a) Left: ISOCAM map, with the LW2 filter (5-8.5 μm), of the bright filament along the western edge of the ρ Ophiuchi main cloud (Abergel et al., 1996). The filament is immersed in the radiation field of the star HD147889 (see the star sign). The four SWS positions (small squares) and the CVF map positions are marked (big squares). (b) Right: ISOCAM-CVF brightness profile of the 0-0 S(3) H_2 line (solid line) and PAH emission (dotted lines) along the cut going through the SWS pointings. **Lower panels.** (a) Left : Pure rotational H_2 lines observed towards the H_2 emission peak of the ρ Oph filament. The line close to 0 shows the rms noise. (b) Right : Excitation diagram (corrected for dust attenuation) for H_2; N_u is the column density of the transition upper level, g_u is the degeneracy of the upper level and T_u is the upper level energy in Kelvin. The solid line is rotational temperature (T_{rot}) thermal distribution for an H_2 ortho-to-para equal at 1.

(χ $\leq$1000, such as Oph W, S140 and IC 63), R_f is about a factor 5 larger than the standard rate estimated in diffuse clouds. On the other hand, towards regions with higher χ (such as NGC 2023 and the Orion Bar), R_f is found to be similar to the standard value. This result can provide at least a partial explanation of the discrepancy discussed above since a larger R_f will move the H^0/H_2 transition zone closer to the edge of the PDR and consequently increase the temperature of the H_2 emitting gas as well as the absolute intensity of the H_2 lines.

This finding of efficient H_2 formation at high gas temperatures ($T_{gas} \geq$ 300 K) has also fundamental implications for our understanding of the H_2 formation process. Since the residence time of weakly bound H atoms on grains (also called physisorbed) at such high temperatures is very short, a process involving strongly bound H atoms is required. An indirect chemisorption process - where a physisorbed H-atom scans the grain surface to recombine with a chemisorbed H-atom (as recently discussed by Cazaux & Tielens, 2002, Cazaux & Tielens, 2003) - is capable of explaining the ISO data (Habart et al., 2004) and could be the most important mechanism in PDRs. Moreover, small grains (radii $<$ a few 10 nm) which dominate the total grain surface and spend most of their time at relatively low (below 30 K for $\chi \leq 3000$) temperatures may be the most promising surface for forming H_2 in PDRs (Habart et al., 2004).

The relationship between aromatic dust particles (referred to as PAHs, radii $<$ 1 nm) and H_2 has been adressed both in the laboratory (Joblin et al., 2001) and observationally (Le Coupanec, 1998; Joblin et al., 2000; An & Sellgren, 2001; Habart et al., 2003; Habart et al., 2004). In particular, using ISOCAM and ground-based observations for a sample of PDRs, Habart et al. (2004) find that the $R_f/[C/H]_{PAH}$ ratio[3] is constant. This suggests, but does not prove, that formation of H_2 on PAHs could be important in PDRs. This result is supported by the observed spatial correlation between the H_2 line emission and the PAH features (see Fig.1 and Le Coupanec, 1998, Joblin et al., 2000, An & Sellgren, 2001, Habart et al., 2003). In the H_2 formation process, very small grains or VSGs (radii between a few nm and a few 10 nm) may also be important (e.g., Boulanger et al., 2004, Rappacioli et al., 2004). In the near future, Spitzer will allow us to examine the VSG emission between 15 and 40 μm towards a number of PDRs and we will be able to better understand the nature of VSGs and to determine their role in the H_2 formation process.

[3] $[C/H]_{PAH}$ is the abundance of carbon locked up in PAHs.

Ortho-to-para H_2 ratio. In several cases, such as the ρ Oph-West (Habart et al., 2003), NGC 2023 (Moutou et al., 1999) or NGC 7023 PDR (Fuente et al., 1999), the H_2 ortho-to-para ratio is significantly smaller than the equilibrium ratio of 3 expected in gas at the temperatures derived from excitation diagrams. This could indicate the presence of (i) dynamical processes, such as the advection of colder gas into the PDR, or (ii) fast conversion of ortho-H_2 to para-H_2 during the formation on the surface of non magnetic, non metallic grains (Le Bourlot, 2000). It must be emphasized here that, as pointed out by Sternberg & Neufeld (1999), care has to be taken with the interpretation of the data since a low ortho/para ratio in excited levels naturally results from the fact that the optical depth in the UV pumping lines is higher for the ortho- than for the para-H_2 lines. Moreover, none of the ISO data measure the bulk of ortho- and para-H_2 which resides in J=0 and 1. We note however that for the physical conditions (χ and n_H) of PDRs discussed here, population of the rotational levels by the cascade following the FUV pumping is generally negligible below S(4) and that the lower lying rotational levels are efficiently populated by collisions. In this latter case, the excitation temperature is well defined and the populations of the $J = 0$ and 1 levels can be derived from a Boltzmann law.

3.2. Shocks

As in the case of PDRs, shocks are luminous sources of H_2. Shocks in molecular clouds can be caused by a large variety of processes including outflows and jets from young stars, supernovae and expanding H II regions (for theoretical reviews see Draine & McKee, 1993, Hollenbach, 1997). In a shock, the mechanical energy is converted into heat and radiated away through cooling lines of atoms and molecules in the IR. For a wide range of shock conditions, H_2 molecules are not dissociated and the gas becomes warm enough for the lowest rotational lines to be excited by collisions.

ISO has detected many lines of H_2 in a number of shocks associated with outflows as Orion OMC-1 (Rosenthal et al., 2000), Cep A West (Wright et al., 1996), DR 21 (Wright et al., 1997), HH 54 (Neufeld et al., 1998), HH 2 (Lefloch et al., 2003), L1448 (Nisini et al., 2000) and also in shocks associated with the supernova remnants IC 443 (Cesarsky et al., 1999), 3C 391, W 44 and W 28 (Rho & Reach, 2003). ISO's main contributions to the study of shocks have been to (i) better characterize the shock structure and physical conditions, especially that found in the slower shocks; (ii) better measure the total cooling power.

The ISO data have also convincingly shown that most of the broad band emission from shocks is due to lines (e.g., Cesarsky et al., 1999). For example, the ISOCAM 7 and 15 μm bands are dominated by the H_2 S(5) and S(1) lines, whereas the IRAS 12, 25, and 60 μm emission is due to H_2 S(2), S(0), and [O I] 63 μm, respectively.

As for PDRs, the pure rotational H_2 transitions dominate the mid-infrared spectra and are characterized by excitation temperatures of T_{ex} ~500-1000 K (see Table 1 and Fig. 2). In contrast, the well-studied H_2 ro-vibrational lines usually yield T_{ex}=2000–3000 K. The most impressive collection of H_2 lines is seen for Orion (see Fig. 2, Rosenthal et al., 2000), where 56 H_2 lines have been seen including the v=0 S(1) to S(25) lines with upper energy levels up to 42,500 K.

Since T_{ex} increases strongly with shock velocity, the observed range of T_{ex} has generally been interpreted in terms of two steady state C-shocks; one with a low density, low velocity (<20 km s^{-1}) and high covering factor to explain the warm, ~700 K, gas, and another with a higher density, higher velocity (30-50 km s^{-1}) and low covering range to explain the hot, ~ 2000 K, gas (e.g., Wright et al., 2000). However, in some circumstances, shocks are unlikely to have attained a state of equilibrium, and a time-dependent approach must be considered. The model of non stationary C-shocks of Pineau Des Forêts & Flower (2000) shows that, at early times, shocks exhibit both C- and J-type characteristics and the existence of both warm and hot components can be explained in terms of a single shock. The H_2 excitation diagram can thus provide a measure of the age of the shock. In the case of the outflow observed in Cep A West (Pineau Des Forêts & Flower, 2000) as well as the supernova remnants IC 443 (Cesarsky et al., 1999), the shocked gas is estimated to have an age of approximately 1.5×10^3 yr.

For most shocks, the inferred ortho/para ratio is 3, consistent with the warm conditions. Major exceptions are HH 54 (Neufeld et al., 1998; Wilgenbus et al., 2000) and HH 2 (Lefloch et al., 2003), where significantly lower ortho/para ratios of 1.2–1.6 are found. This low ratio is thought to be a relic of the earlier cold cloud stage, where the timescale of the shock passage was too short to establish an equilibrium ortho/para ratio. Thus, the ortho/para ratio can be used as a chronometer, indicating for HH 54 that the gas has been warm for at most 5000 yr.

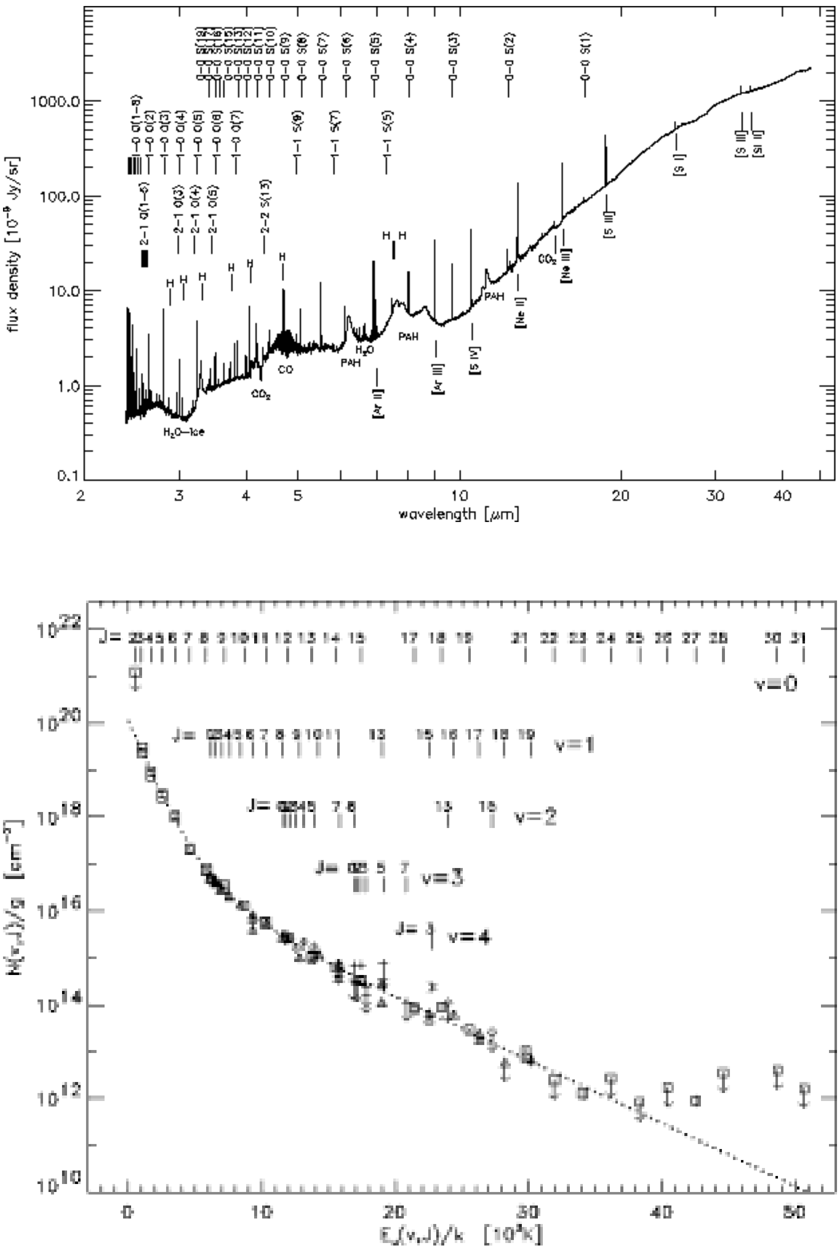

Figure 2. Upper panel: SWS spectrum towards the brightest H_2 emission peak of the Orion OMC-1 outflow of Orion Peak 1 showing a multitude of ro-vibrational and pure rotational lines (Rosenthal et al., 2000). Lower panel: Excitation diagram (corrected for dust attenuation) for H_2; for the lowest energy levels the excitation temperature is about 600 K whereas at $E(v, J)/K$ ≥14,000 K it is about 3000 K.

3.3. Circumstellar environment of YSOs

H_2 is expected to be ubiquitous in the circumstellar environment of Young Stellar Objects (YSOs). It is the main constituent of the molecular cloud from which the young star is formed and is also expected to be the main component of the circumstellar disk. Most of this material however is at low temperatures and the pure rotational lines are difficult to observe. However, certain zones may be heated to temperatures of a few hundred K and produce observable H_2. The intense UV radiation generated by accretion as well as that from the central star itself creates a PDR in the surrounding material. Another way of producing warm H_2 is in shocks caused by the interaction of an outflow with the surrounding molecular cloud or envelope.

Intermediate- and high-mass YSOs : from shocks to PDRs. van den Ancker et al. (2000a; 2000b) have studied H_2 emission in a sample of 21 YSOs mostly of intermediate- and high-mass. Pure rotational H_2 emission was detected in 12 sources. In Fig. 3, we show the excitation diagrams of some sources at different stages of evolution. To determine the excitation mechanisms responsible for the H_2 emission, van den Ancker et al. (2000a; 2000b) compare these observations to PDR and shock models. However, for the physical conditions prevailing in these objects, there is generally a considerable overlap between the temperatures predicted by the different models. Thus, van den Ancker et al. (2000a; 2000b) use additional tracers, such as PAH emission - indicative of the presence of a PDR - or [SI] 25.25 μm emission indicative of shocks. They find that the H_2 lines of the embedded sources originate from shocks, whereas more evolved objects are characterised by H_2 lines from a PDR. As the envelope disperses, the PDR component starts to dominate compared to the shock emission.

Circumstellar disks. Deep searches for the H_2 S(0) and S(1) lines at 28 and 17 μm have been performed with the SWS towards a dozen young stars (Thi et al., 2001). Detections have been claimed in several sources but contamination from surrounding cloud material can be important (e.g., Richter et al., 2002). Recently, using TEXES/IRTF with higher spectral ($\lambda/\Delta\lambda \sim 80,000$ at 12.3 μm) and spatial resolution (0.85" at 12.3 μm), Richter et al. (2004) have detected the H_2 S(1) and S(2) lines in circumstellar disks around several Herbig Ae and T Tauri stars. Preliminary analysis suggests that the gas temperatures are between 400 and 800 K. This is consistent with recent FUSE observations of two Herbig Ae stars, namely HD100546 and HD163296, suggesting the presence of dense and warm ($\sim$400-700 K) H_2 in the circumstellar disks (Lecavelier des Etangs et al., 2003). In the near

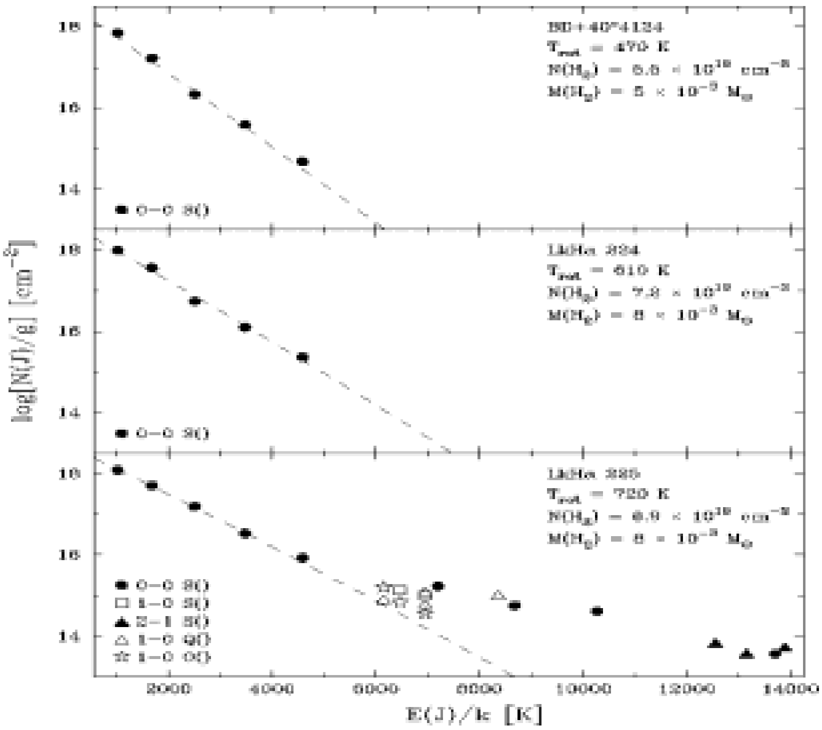

Figure 3. Excitation diagrams (corrected for dust attenuation) for H_2 of young intermediate-mass stars in the BD $+40^o4124$ group (van den Ancker et al., 2000b). ¿From bottom to top, we find in a rough evolutionary sequence LkHα 225, LkHα 224 and BD $+40^o4124$.

future, observations from Spitzer and VISIR, accompanied by more sophisticated modelling, should be able to clarify the origin of the H_2 emission from disks.

3.4. Planetary Nebulae and PPN

H_2 is also an important component of the neutral material of envelopes expanding away from the hot central stars of Planetary nebulae (PNe). In these objects, the H_2 emission may originate in the shock between the shell and the wind of the precursor red giant or in the PDR on the inside of the neutral shell. Moreover, the H_2 excitation mechanism is expected to change with time (e.g., Natta & Hollenbach, 1998). Presently, the largest body of evidence comes from observations of the H_2 2 μm fluorescent transitions. The morphology and excitation of the H_2 fluorescent emission in AFGL 2688 and NGC 7027 are, in particular, consistent with an evolutionary scheme in which shock excitation dominate in the proto-planetary nebula (PPN) phase and FUV excitation from PDRs dominate in young PNe (e.g., Cox et al., 1997).

ISO allowed us to observe several rotational and ro-vibrational lines of H_2 from PPN (such as CRL 618, Herpin et al., 2000), young nebulae (such as NGC 7027, Bernard Salas et al., 2001), and fully evolved PNe (such as the Helix or the Dumbbel, Cox et al., 1998, Bachiller et al., 2000). Analysis of these data brings new perspectives on the different possible H_2 excitation mechanisms at different evolutionary stages of PNe. As an illustration, we discuss in the following two extreme cases, namely the proto-planetary nebula CRL 618 and the evolved Helix nebula.

The PPN CRL 618. Many rotational and ro-vibrational lines of H_2 were detected by ISO-SWS towards the proto-planetary nebulae CRL 618 (Herpin et al., 2000). The analysis of these data shows that shocks in the lobes may collisionally excite the lowest pure rotational emission whereas the highest transitions ($v \geq 2$) may come from fluorescence in the torus. A mix of fluorescence and collisions may produce the $v = 1$ to 0 transitions in an intermediate zone. Recent high spatial and spectral resolution spectro-imaging of the H_2 1-0 S(0) line using BEAR reveal the presence of multiple, high-velocity, molecular outflows that align with the optical jets, and show how jets interact with circumstellar gas and shape the environment in which planetary form (Cox et al., 2003).

The Helix. In the Helix, an evolved PNe, a detailed study of the H_2 rotational lines (Cox et al., 1998) has been carried out with ISOCAM data. The CVF spectro-imaging data shows that the mid-IR emission is entirely caused by H_2 and neon lines (see Fig. 4); no dust bands are detected and the continuum emission is very weak. The H_2 emission traces the individual cometary globules of the molecular envelope of the nebula (see Fig. 4). Despite the fact that the globules in the Helix show a typical PDR morphology, Cox et al. (1998) conclude that the far-UV radiation from the central star is of much too low intensity ($\chi \sim 6$) to account for the H_2 line intensities and high temperatures (900 K) that are observed. The extreme-UV radiation from the star could perhaps play an important role in heating the H_2 if it survives up to the ionization front. Time-dependent calculations including the effects of rapid changes in the stellar effective temperature, χ and n_H

as well as the advance or retreat of the ionization front with respect to the PDR gas are needed to better understand the physics of PNe. Comparison with future H_2 observations at high angular resolution should help to further constrain the excitation of H_2 in PNe.

3.5. Galactic center region and diffuse galactic medium

ISO has also provided some clues in our understanding of warm gas in the galactic center region as well as in the diffuse interstellar medium.

Warm H_2 in the Galactic center region. Several pure-rotational lines have been observed towards a sample of molecular clouds distributed along the central 500 pc of the Galaxy (Rodriguez-Fernandez et al., 2001). The S(0) and S(1) lines trace gas with temperatures of 150 K while the S(4) and S(5) lines indicate temperatures of 600 K. The 150 K-H_2 column density is typically 1-2 10^{22} cm^{-2}. This is the first direct estimate of the total column density of the warm molecular gas in the Galactic center region. These warm column densities represent a fraction of 30% of the gas traced in CO. In order to explain all the observed H_2 lines, Rodriguez-Fernandez et al. (2001) find that a combination of both high and low density PDRs or shocks is required. Moreover, non-equilibrium ortho-to-para ratios have been found in two clouds of the sample suggesting heating by low velocity shocks ($\sim$ 10 km s^{-1}, Rodriguez-Fernandez et al., 2000).

Hot gas in the cold diffuse medium. Most of the diffuse interstellar medium is cold, but it must have pockets of hot gas to explain the large observed abundance of molecules like CH^+, OH and HCO^+. To test the existence and determine the characteristics of this component, Falgarone et al. (2000) have searched using ISO-SWS for H_2 rotational lines along a line of sight close to the galactic plane, carefully avoiding star forming regions and molecular clouds. The intensities of the S(2) and S(3) lines are about one order of magnitude above those predicted by radiative excitation. This result suggests the existence of a small fraction (few %) of hot (a few 100 K) gas in the cold interstellar medium and for which UV photons cannot be the sole heating source. The possible excitation process could be the deposition of mechanical energy in shocks or in vortices formed by the viscous dissipation of turbulence (see in this review the chapter on the cool interstellar medium by Abergel et al.).

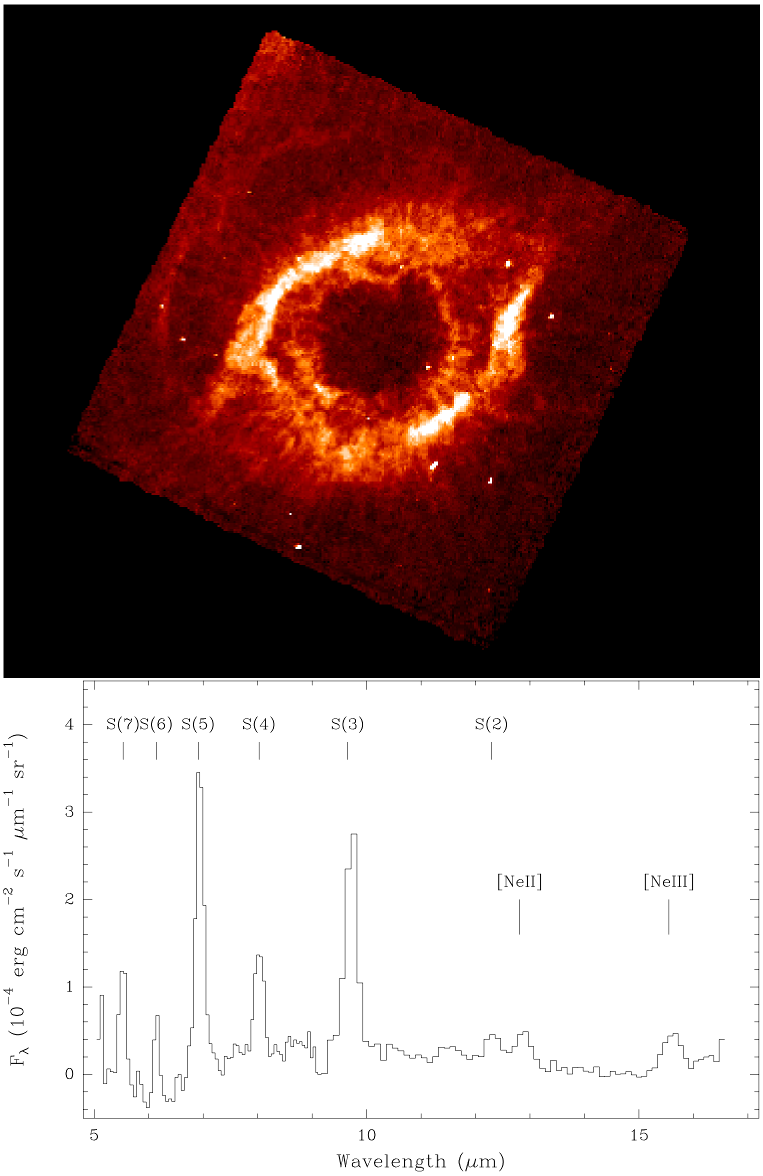

Figure 4. Upper panel: An ISOCAM map of the Helix Planetary Nebula in the LW2 filter dominated by the strong 0-0 S(5) H_2 line (Cox et al., 1998). Lower panel : CVF spectra toward the H_2 emission peak in the western rim of the Helix nebula.

3.6. Extragalactic sources

Prior to ISO, H_2 emission in external galaxies was detected in the near-IR ro-vibrational lines, from typically 10^4 $M_\odot$ of H_2 heated to temperatures of ~2000 K, in the centers of starburst, active and (ultra)luminous infrared galaxies. However, gas at these temperatures is a very small fraction (10^{-6}) of the total amount of H_2 gas (e.g., van der Werf et al., 1993).

ISO-SWS offered the unique opportunity to detect pure rotational H_2 emission in various galaxies, from normal to ultraluminous, and thus to study the amount of warm ($T \gtrsim 80$) gas in these galaxies (e.g., Valentijn et al., 1996, Valentijn & van der Werf, 1999, Genzel & Cesarsky, 2000, Rigopoulou et al., 2002, Lutz et al., 2003). These observations provide unique probes of the various heating mechanisms. For instance, in starburst galaxies, H_2 emission may be generated by UV-pumping in star-forming regions or by shocks due to outflows, supernova remnants or large-scale streaming motions in spiral arms and bars; in addition X-ray excitation may be produced by multiple supernovae remnants or by an active galactic nucleus or cooling flow.

Normal galaxies. The first extragalactic detection of the 0-0 S(0) and S(1) lines in the center of the nearby Scd galaxy NGC 6946 revealed 5 10^6 $M_\odot$ of warm, (T=170 K) circumnuclear gas (Valentijn et al., 1996). Radiation from massive stars or shocks from e.g. supernovae explosions in the nuclear complex are the most obvious mechanisms for producing this warm component. Throughout the disk of the edge-on spiral galaxy NGC 891, such warm H_2 components have also been detected (Valentijn & van der Werf, 1999). Additionally, a cooler T_{gas} ~80 K component was observed in the outer disk. This can most likely be identified with extended low-density PDRs which form the warm envelopes of giant molecular clouds, heated by the local interstellar medium. Moreover, this component may harbour a very significant mass and the implications for the galactic mass budget have been explored by Valentijn & van der Werf (1999). This finding might provide a solution to the missing mass problem.

Starburst and Seyfert galaxies. Using ISO-SWS, Rigopoulou et al. (2002) has performed a survey of H_2 emission from active galaxies displaying a wide range in nuclear activity including starburst and Seyfert galaxies. A number of transitions from 0-0 S(0) to S(7) are detected in both starbursts and Seyferts. The data reveal different components at different temperatures. The temperature of the more abundant warm gas - probed by the S(0) and S(1) lines - is similar in starbursts and Seyferts with a value of around ~150 K. This warm gas accounts for as much as 10% of the total galactic gas mass in starbursts and up to 35% in Seyferts. Also, by comparison with model predictions, Rigopoulou et al. (2002) find that a combination of various PDRs could explain the line ratios observed in starbursts. Although such a combination of PDRs can also match the observations in Seyferts, it is likely that shocks and heating from the central X-ray source are also present. This is confirmed by the observed H_2/PAH emission ratio. In fact, in starbursts and Seyferts with a strong starburst component, Rigopoulou et al. (2002) find that the PAH and H_2 emission are well correlated implying that these emissions have a common starburst origin. On the other hand the H_2/PAH emission ratio is higher in pure "AGN-dominated" objects suggesting the presence of an extended circumnuclear component of warm gas heated by the nuclear X-ray emission in which the enhanced H_2 emission originates. This warm gas component is either too far away for UV photons to reach or, acts as a shield to UV photons resulting in both cases in suppressed PAH emission.

4. Conclusions and future prospects

ISO provided a fundamental step forward in that it enabled us for the first time to exploit the potential of the pure rotational series of H_2. It was possible to estimate temperatures and densities in the important transition layers of the ISM separating neutral and ionised gas. Such measurements also allowed estimates of the H_2 formation rate on grain surfaces and suggested that molecular hydrogen might preferentially be formed on PAHs and/or very small grains. ISO H_2 data also allowed us to better characterize the shocks associated with outflows from young stars or supernova remnants. H_2 lines can in particular be used to estimate the age of the shock. Moreover, new insights into the different possible H_2 excitation mechanisms at different evolutionary stages of young stellar objects and planetary nebulae have been obtained. ISO also gave us for the first time the possibility to observe the pure rotational lines of H_2 in galaxies, from normal to ultraluminous. This permitted the study of the amount of warm ($T \gtrsim 80$ K) gas in these galaxies and provided unique probes of the dominant heating mechansims (photon heating, shock, X-ray).

An obvious question is that of what one can expect from future space missions as well as from the use of modern spectrometers on large ground based instruments. It is perhaps worth stressing that our present capacity to use infrared observations of H_2 as a probe of interstellar (galactic and extragalactic) conditions is limited by a variety of factors including sensitivity but also spatial and spectral resolution. The importance of high spatial resolution is made clear both by ground based images in the 2 μm 1-0 S(1) line as well as by the difficulties encountered both from the ground and space in separating diffuse emission and emission from point sources in crowded fields. Hardly less important is high spectral resolution both because of the kinematic information which becomes available for $R = \lambda/\Delta\lambda$ greater than 10,000 and because of the problems of blending of weak spectral features.

The IRS instrument on Spitzer covering the 5-40 μm range is already demonstrating the advantages of increased sensitivity for the study of H_2 lines in young star forming regions (e.g., Morris et al., 2004) and galaxies (e.g., Smith et al., 2004, Armus et al., 2004). Spitzer will extend medium resolution spectroscopy of H_2 lines into regimes that ISO could not probe, and will provide a large number of new targets for further works.

Sensitive ground based studies are already possible with ISAAC at the VLT (wavelength range 1-5 μm, $R \sim$1000-10,000) but the future presumably belongs to CRIRES/VLT (wavelength range 1-5 μm, $R \sim$20,000-100,000). CRIRES will allow the observation of high J H_2 rotational transitions as well as a variety of ro-vibrational lines with both high spectral and spatial resolution. In addition, VISIR/VLT will permit at longer wavelengths observation of the 0-0 S(1) and S(3) H_2 transitions with a spatial resolution of ~0.3" and $R \sim$20,000 at 10 μm. Of course, the sensitivity of these ground based instruments is limited by the atmosphere and thus the insight gained by such measurements (relative say to ISO) will be greatest for stellar and other compact sources of H_2 emission. The potential of such high resolution ground based instruments has already been demonstrated by the results from the TEXES/IRTF spectrometer (5-25 μm, $R \sim 100,000$) observing the rotational transitions of H_2 in disks (Richter et al., 2004) and the Orion Bar (Allers et al., 2004).

Such ground based instruments are hopefully the forerunners of high class instrumentation in space or from airborne platforms. The spectrometers on SOFIA (covering 0.3-1600 μm) will soon observe several H_2 lines including the 28 μm S(0) transition with diffraction limited resolution of 1.5" and $R \sim 10^4 - 10^5$ at 20 μm. In the long term, MIRI on JWST (5-28 μm, ~0.1" of spatial resolution) will allow high class maps of the H_2 rotational transitions and comparisons with the 2 μm 1-0 S(1) maps. The combination of these instruments will be very powerful and it will become a challenge for theorists to understand the images they produce.

Table I. Sample of ISO H_2 observations in various astrophysical objects

		PDRs			shocks		YSOs	
objects	Oph W	IC 63	Orion Bar	Orion Pk1	Cep A W	IC 443	LkHα225	BD+40^{o}4124
n_H (cm^{-3})	10^4	0.5-1 10^5	0.5-3 10^5	10^5-10^6	10^4-10^6	10^4	10^5	10^4-10^6
χ^a	250	650	0.5-2.4 10^4					10^4-10^5
T^b_{rot} (K)	330	620	390	630	688	500	720	470
$N^c_{H_2}$ (10^{21} cm^{-2})	0.6	5	1	1.4	0.18	0.1-1	0.069	0.055
Ref.	1	2	3	4	5	6	7	7

	PPN	PNe	Galactic center	normal galaxy		starbursts	Seyferts
objects	CRL 618	Helix		NGC 6946	NGC 891-outer disk		
n_H (cm^{-3})	10^6-10^7	$\geq 10^5$	10^3-10^6	10^2-10^5	10^2-10^5	10^3-10^6	10^3-10^6
χ^a		4	10^3-10^6				
T^b_{rot} (K)	750	900	150	170	80	150	150
$N^c_{H_2}$ (10^{21} cm^{-2})	68	0.003	10-20	23	100	1-100	1-100
Ref.	8	9	10	11	12	13	13

[a] Incident FUV radiation field expressed in units χ of the Draine (1978) average interstellar radiation field.
[b] Excitation temperature of the low H_2 pure rotational levels.
[c] H_2 column density inferred from the intensity of H_2 rotational lines and assuming that the population distribution of low H_2 rotational levels is essentially in LTE.
References. (1) Habart et al. (2003); (2) Thi et al. (1999) (note that the observations cannot be fitted by a single excitation temperature but two components at ∼100 K and ∼620 K are needed) and Jansen et al., Jansen et al. (1994, 1995); (3) data from Bertoldi, priv. com. and see references in Habart et al. (2004); (4) Rosenthal et al. (2000); (5) Wright et al. (1996); (6) Cesarsky et al. (1999); (7) van den Ancker et al. (2000b); (8) Herpin et al. (2000); (9) Cox et al. (1998); (10) Rodriguez-Fernandez et al. (2001); (11) Valentijn et al. (1996); (12) Valentijn & van der Werf (1999); (13) Rigopoulou et al. (2002).

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