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H_2 in Space

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Abstract. Molecular hydrogen may be excited by collisions with other particles (as in shock waves), by ultraviolet pumping (as in photon-dominated regions), through its formation on the surfaces of dust grains (in interstellar clouds), or by absorption of the cosmic background radiation (in the primordial gas). We consider the adequacy of our knowledge of H_2, from the viewpoint of being able to reliably predict the spectrum arising from these excitation mechanisms.

1. Shocks in molecular outflows

Low-mass star formation is known to be accompanied by jets of outflowing material which impact the surrounding gas at supersonic speeds. Shock waves are produced, both in the jet and in the ambient molecular gas, and the associated compression and heating give rise to excitation of H_2 molecules. Vibrational transitions of H_2 from outflow sources have been observed for a number of years, through atmospheric windows in the near infrared (Gredel 1994, 1996), but the advent of ISO enabled pure rotational transitions to be observed also (Wright et al. 1996). These radiative transitions of H_2, observed in emission, contribute to the *cooling* of the medium. The interpretation of their intensities requires a knowledge of the rate coefficients for collisional excitation of rovibrational transitions of H_2 (Flower et al. 2000).

C-type shock waves generated in outflows will not have attained steady state, in view of the short dynamical timescales (of the order of 10^3 yr) which are associated with the jets (Pineau des Forêts & Flower 2000). Time-dependent MHD calculations show that a shock wave evolves from J- to C-type over a period of about 10^4 yr, under the physico-chemical conditions appropriate to molecular outflows. At intermediate times, of the order of 10^3 yr, the shock wave possesses both J- and C-type character (Chièze et al. 1998). Only at this stage in the shock wave's evolution can the distribution of population amongst the rotational levels of H_2, observed in Ceph A by Wright et al. (1996), be successfully reproduced by the model.

2. Photon-dominated regions

PDR's arise when high-mass stars form and begin to radiate in the ultraviolet. The remnants of the cloud from which the stars have contracted are then exposed to a radiation field which can be orders of magnitude more intense than the local interstellar background field.

The well-known reflection nebula NGC 2023 has been modelled by Draine & Bertoldi (2000), who found that the PDR has a density of 5×10^4 cm^{-3}, is seen almost edge-on, and is exposed to a radiation field which is 5000 times the local interstellar background. ISO observations of emission lines within the vibrational ground state of H_2 can be reproduced up to rotational level $J = 15$ – although a scaling factor has to be introduced in order to obtain agreement with the absolute line intensities. Draine & Bertoldi (2000) conclude that there is an approximate balance between photodissociation of H_2 by ultraviolet radiation and the formation of H_2 on grains. This latter process may also contribute significantly to the intensities of emission lines from high J levels. In the PDR context, collisions with H_2 molecules can *heat* the gas, by de-exciting vibrational states which have been populated by absorption of radiation.

3. The primordial gas

H_2 and its deuterated analogue, HD, were present in the primordial gas, the concentration of the latter being enhanced by chemical fractionation. The formation of the first gravitationally bound structures was mediated by H_2 and HD cooling of the gas, through collisional excitation followed by radiative decay.

The temperatures of matter T_m and of radiation T_r in the homogeneous and uniformly expanding primordial medium decoupled at a redshift $z \approx 300$, beyond which $T_r > T_m$. However, even for $z < 300$, the populations of the rotational levels of ortho- and para-H_2 continued to be thermalized by the blackbody radiation field. The ortho:para ratio, on the other hand, is determined by proton-exchanging collisions with residual H^+ in the gas. Collisions between H_2 molecules and, principally, protons result in *heating* of the gas, through de-excitation of rotationally excited states of H_2. Neglect of proton collisions leads to the rate of this heating process being underestimated by large factors (Flower & Pineau des Forêts 2000).

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