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THE EMISSION SPECTRUM OF H_2 FROM ASSOCIATIVE DETACHMENT AND ULTRAVIOLET PUMPING

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ABSTRACT

The infrared emission spectrum of H_2 resulting from the associative detachment of H and H^- is calculated. It is characterized by pure rotational transitions in excited vibrational states and is readily distinguished from that expected from ultraviolet pumping or from shock excitation. The combined effects of associative detachment and of ultraviolet pumping are discussed with reference to H_2 line emission from planetary nebulae.

Subject headings: infrared: spectra — masers — molecular processes — nebulae: planetary

I. INTRODUCTION

Molecular hydrogen has been detected in several planetary nebulae (Treffers *et al.* 1976; Beckwith, Persson, and Gatley 1978; Smith, Larson, and Fink 1981) by observations of infrared emission lines originating in the first two excited vibrational levels, $v = 1, 2$. Black (1978) has discussed molecule formation in the transition zones of planetary nebulae in which associative detachment,

$$H + H^- \rightarrow H_2 + e\ , \qquad (1)$$

(McDowell 1961; Dalgarno and McCray 1973) is a principal source of H_2. In such circumstances, rotation-vibration transitions can be excited by collisions, by ultraviolet pumping (Black and Dalgarno 1976), and by the formation process itself.

Ultraviolet pumping gives rise to a spectrum dominated by transitions from levels with small values of the rotational quantum number J. In contrast, the formation process represented in equation (1) initially populates levels with high values of v and J (Bieniek and Dalgarno 1979), and the subsequent cascading produces a characteristic emission spectrum.

We calculate here the emission spectrum of H_2 resulting from associative detachment, and we explore its modification by ultraviolet pumping. H_2 is also formed by association reactions on grain surfaces and by reaction of H_2^+ with H,

$$H_2^+ + H \rightarrow H_2 + H^+\ . \qquad (2)$$

The H_2^+ ions may be formed by radiative association,

$$H + H^+ \rightarrow H_2^+ + h\nu\ . \qquad (3)$$

II. THEORY

a) The Spectrum due to Associative Detachment

Associative detachment,

$$H + H^- \rightarrow H_2(v, J) + e\ , \qquad (4)$$

populates excited vibration-rotation levels (v, J) of H_2. The individual rate coefficients $k(v, J)$ have been calculated by Bieniek and Dalgarno (1979) and by Bieniek (1980) for temperatures of 100 K, 1000 K, and 5000 K. The newly formed, excited molecules undergo a cascade through lower levels, terminating in the ground vibrational state. The cascading paths are determined by the radiative probabilities of the possible quadrupole transitions (Turner, Kirby-Docken, and Dalgarno 1977).

We have followed the procedures of Black and Dalgarno (1976), extended to higher values of J, to follow the cascading, and we have computed the resulting emission spectrum. The emission is distributed over many lines, the strongest of which lie between 3.4 μm and 5.0 μm. The strongest transitions at 1000 K and 5000 K and their emissivities are listed in Table 1. The strongest transitions at 5000 K in the wavelength region $\lambda \leq 2.5\ \mu$m are listed in Table 2. The emissivity due to associative detachment in a transition $(v', J') \rightarrow (v'', J'')$ may be written in photons cm^{-3} s^{-1} in the form

$$j(v', J'; v''J'') = 2 \times 10^{-9} n(\mathrm{H}) n(\mathrm{H}^-) \epsilon(v'J'; v''J'')\ , \qquad (5)$$

where $n(\mathrm{H})$ and $n(\mathrm{H}^-)$ are the concentrations of H and H^- respectively in cm^{-3} and ϵ is the relative emissivity (photons emitted per molecule formed), presented in Tables 1 and 2. The spectra at 1000 K and 5000 K differ in their detailed structure, but both are characterized by strong, pure rotational transitions between levels of high J in vibrational levels $v = 1$, 2, and 3. The radiative cascade following associative detachment produces a total of 3.4–3.8 infrared photons per molecule formed.

The strongest lines in Table 1 appear near a wavelength of 4μm. It is instructive to compare these emissivities with that of the neighboring H Brα line, λ4.052 μm, which has been detected in several nebulae. To obtain estimates of the intensity ratios, we ignore the details of the ionization structure near the boundary and adopt a model of the transition zone of thickness δr in which $n(e) = n(\mathrm{H}) = 0.5n$.

The formation of H_2 by associative detachment is efficient where free electrons and neutral H atoms exist in

TABLE 1

Relative Emissivities ϵ of the Strongest Infrared Lines Produced by Associative Detachment

Transition	$\lambda(\mu m)$	ϵ
$T = 5000$ K		
1–1 $S(13)$	3.992	0.1211
1–1 $S(15)$	3.666	0.1147
1–1 $S(11)$	4.390	0.1114
2–2 $S(15)$	3.900	0.1037
2–2 $S(17)$	3.567	0.0952
2–2 $S(13)$	4.241	0.0905
1–1 $S(17)$	3.350	0.0860
1–1 $S(9)$	4.948	0.0729
2–2 $S(11)$	4.656	0.0611
3–3 $S(15)$	4.138	0.0432
1–0 $S(7)$	1.748	0.0412
3–3 $S(17)$	3.788	0.0411
1–1 $S(14)$	3.824	0.0383
1–1 $S(12)$	4.177	0.0381
1–1 $S(16)$	3.510	0.0354
Total		3.787
$T = 1000$ K		
2–2 $S(13)$	4.241	0.0785
2–2 $S(15)$	3.900	0.0751
1–1 $S(11)$	4.390	0.0743
1–1 $S(13)$	3.992	0.0662
2–2 $S(11)$	4.656	0.0594
1–1 $S(9)$	4.948	0.0578
3–3 $S(15)$	4.138	0.0527
1–1 $S(15)$	3.666	0.0475
3–3 $S(13)$	4.495	0.0466
2–2 $S(17)$	3.567	0.0461
3–3 $S(17)$	3.788	0.0419
1–0 $S(7)$	1.748	0.0393
1–0 $S(5)$	1.836	0.0354
Total		3.388

comparable concentrations. The negative ion forms by radiative attachment,

$$H + e \rightarrow H^- + h\nu \,, \tag{6}$$

and is removed by the reaction represented in equation (1), by photodetachment,

$$H^- + h\nu \rightarrow H + e \,, \tag{7}$$

and by mutual neutralization,

$$H^- + H^+ \rightarrow H + H \,, \tag{8}$$

(see Dalgarno and McCray 1973). The rate coefficients at $T = 5000$ K of reactions (1), (6), and (8) are 2×10^{-9}, 2.55×10^{-15}, and 5.7×10^{-8} cm^3 s^{-1} respectively. In the optimal circumstance when $n(e) = n(H) = 0.5n$, and reaction (7) can be neglected,

$$n(H^-) = 2.2 \times 10^{-8} n \tag{9}$$

and the emissivity is given by

$$j(v'J';\, v''J'') = 2.2 \times 10^{-17} n^2 \epsilon(v'J';\, v''J'') \,. \tag{10}$$

In a fully ionized, spherical nebula of radius r_0, the luminosity in a line of H_2 formed in the transition zone is related to the luminosity of H Brα by

$$\frac{L_{H_2}}{L_H} = 6.54 \times 10^{-17} \frac{\delta r}{r_0} \frac{\epsilon}{\alpha_{54}} \left(\frac{4.052}{\lambda}\right) , \tag{11}$$

where λ is the wavelength of the H_2 line in μm and α_{54} is the effective recombination coefficient for production of the hydrogen Brα photons. Values of α_{54}, derived from the calculations of Brocklehurst (1971) and Giles (1977) for case B recombination, are given in Table 3. If the entire nebula is observed, equation (11) is equivalent to the intensity ratio. For a nebula of temperature 10^4 K and density 10^4 cm^{-3} with a transition zone at a temperature around 5000 K, the relative intensities of the strongest of the H_2 lines, the 1–1 $S(13)$ line at 3.992 μm, and Brα are given by $I(3.992)/I(4.052) = 0.028(\delta r/r_0)$.

For the planetary nebula NGC 7027, we may use the measured intensity of H Brγ (Smith, Larson, and Fink 1981) in conjunction with recombination theory to predict that $I(4.052) = 1.6 \times 10^{-10}$ ergs cm^{-2} s^{-1}. The predicted intensity is consistent with the lower limit obtained by Merrill, Soifer, and Russell (1975). The 1–0 $S(1)$ line at 2.122 μm has been observed in NGC 7027

TABLE 2

Relative Emissivities of the Strongest Short-Wavelength ($\lambda < 2.5$ μm) Lines Produced by Associative Detachment at $T = 5000$ K

Transition	$\lambda(\mu m)$	ϵ
1–0 $Q(1)$	2.407	0.00959
1–0 $Q(3)$	2.424	0.01108
1–0 $S(1)$	2.122	0.01382
1–0 $Q(5)$	2.455	0.01212
1–0 $S(3)$	1.958	0.02002
1–0 $Q(7)$	2.500	0.01748
1–0 $S(5)$	1.836	0.02954
1–0 $S(6)$	1.788	0.01217
1–0 $S(7)$	1.748	0.04117
1–0 $S(8)$	1.715	0.01222
1–0 $S(9)$	1.688	0.02796
2–1 $S(5)$	1.945	0.01075
2–1 $S(7)$	1.853	0.01273
2–1 $S(9)$	1.791	0.01013
2–1 $S(15)$	1.710	0.01200
2–1 $S(17)$	1.688	0.02437
3–2 $S(15)$	1.815	0.01513
3–2 $S(17)$	1.790	0.02565
4–3 $S(15)$	1.972	0.01344
4–3 $S(17)$	1.963	0.01836
5–4 $S(15)$	2.127	0.01111
5–4 $S(17)$	2.116	0.01060
2–0 $S(7)$	1.064	0.01278
2–0 $S(9)$	1.054	0.02121
2–0 $S(11)$	1.053	0.02167
2–0 $S(13)$	1.061	0.01409
3–1 $S(7)$	1.130	0.01079
3–1 $S(9)$	1.120	0.01532
3–1 $S(11)$	1.119	0.01673
3–1 $S(13)$	1.126	0.01169
4–2 $S(9)$	1.195	0.01009
4–2 $S(11)$	1.197	0.01011

TABLE 3

EFFECTIVE RECOMBINATION COEFFICIENTS α_{54} FOR H Brα (case B) (10^{-16} cm^3 s^{-1})

T	$n(e)$: 0	10^2	10^4	10^6
5000	7.155	6.673	6.487	5.925
10,000	3.061	2.872	2.836	2.673

(Smith, Larson, and Fink). For our simplified model with $\delta r/r_0 = 0.1$, we estimate an intensity $I(2.122) = 7.1 \times 10^{-14}$ ergs cm^{-2} s^{-1} arising from the population by associative detachment. The observed intensity is at least an order of magnitude larger, and the formation mechanism is not a sufficient source. Ultraviolet pumping (Black and Dalgarno 1976) will enhance the population, and, in our further calculations, we have included its contribution.

b) The Effects of Ultraviolet Pumping

To explore the effects of ultraviolet pumping, we assumed that the populations of the excited vibrational levels are determined by the H_2 formation process and by ultraviolet pumping from the ground vibrational level, $v = 0$. We assumed that the rotational distribution in the $v = 0$ level is determined by ultraviolet pumping, radiative decay, and collisions with electrons and neutral hydrogen atoms.

We obtained the rate coefficients for the electron impact excitation of the $J = 0 \rightarrow 2$ transition from the cross sections measured by Crompton, Gibson, and McIntosh (1969) and Linder and Schmidt (1971), and we used a theoretical scaling law for other transitions (see Chang and Temkin 1969; Klonover and Kaldor 1978; Chang 1981). For the rate coefficients for rotational energy transfers in collisions with hydrogen atoms, we adopted the formula developed by Elitzur and Watson (1978) to represent the available quantal calculations. Considerable uncertainty still remains in the rate coefficients (Green and Truhlar 1979), but, in the plasma environment, electron collisions are usually more efficient.

We adopted an ionizing source characterized by a blackbody radiation field at a temperature of 10^5 K with a short-wavelength cut-off at the Lyman limit. The rates of entry $\mu(v, J)$ cm^{-3} s^{-1} into levels (v, J) through ultraviolet pumping of the $(0, J'')$ levels are readily calculated (Black and Dalgarno 1976). The (v, J) levels then cascade down, ultimately populating the rotational levels of the ground vibrational level $v = 0$.

In Table 4, we present the calculated values of the probabilities p_{ij} which are the fraction of the absorption by level $J = i$ that terminates in level $J = j$ of $v = 0$. The difference between unity and $\sum_j p_{ij}$ is the fraction that leads to dissociation. The dissociation efficiency is about 8.7% for each photon absorbed so that the total pumping rate is about 12 times the photodissociation rate. The dissociation efficiency is smaller than that appropriate to the interstellar radiation field because the harder ionizing spectrum of the central star enhances the probability of absorption into the upper $C\ ^1\Pi_u$ state of the Werner system, from which spontaneous radiative dissociation is less probable (Stelphens and Dalgarno 1972).

If reaction (1) is the only source of molecular hydrogen and fluorescent photodissociation the only sink, the entry rate into level (v, J) may be written

$$R(v, J) = kn(\mathrm{H})n(\mathrm{H}^-) \times \left[\frac{k(v, J)}{k} + \frac{12\mu(v, J)}{\mu}\right] \mathrm{cm}^{-3}\ \mathrm{s}^{-1}\ , \quad (12)$$

where

$$k = \sum_{v,J} k(v, J) \approx 2 \times 10^{-9} \quad (13)$$

and

$$\mu = \sum_{v,J} \mu(v, J)\ . \quad (14)$$

The equilibrium population of state $(v > 0, J)$ is given by

$$n(v, J) = \left[R(v, J) + \sum_{v' \geq v} \sum_{J'} n(v', J')A(v'J'; vJ)\right] \Big/ A(vJ)\ , \quad (15)$$

where the $A(v'J'; vJ)$ are spontaneous transition probabilities (Turner, Kirby-Docken, and Dalgarna 1977), and

TABLE 4

VALUES OF THE PROBABILITIES p_{ij} FOR A BLACKBODY RADIATION FIELD AT A TEMPERATURE OF 10^5 K WITH NO PHOTONS WITH WAVELENGTHS LESS THAN 911.7 Å

i/j	0	1	2	3	4	5	6	7	8	9	10
0	0.196		0.443		0.195		0.038		0.003		0.000
1		0.406		0.350		0.103		0.014		0.001	
2	0.126		0.444		0.246		0.050		0.005		0.000
3		0.279		0.400		0.167		0.025		0.002	
4	0.081		0.323		0.336		0.116		0.013		0.001
5		0.182		0.312		0.282		0.086		0.007	
6	0.048		0.217		0.288		0.245		0.067		0.004
7		0.103		0.225		0.265		0.218		0.056	
8	0.022		0.123		0.227		0.247		0.200		0.048
9		0.043		0.138		0.231		0.231		0.184	
10	0.007		0.054		0.155		0.236		0.213		0.170

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TABLE 5

COMBINED EFFECTS OF ASSOCIATIVE DETACHMENT AND ULTRAVIOLET PUMPING

TRANSITION	$\lambda(\mu m)$	ϵ	
		$T = 5000$	$T = 1000$
1–1 $S(13)$	3.992	0.1248	0.06667
2–2 $S(15)$	3.900	0.1041	0.07517
3–3 $S(15)$	4.138	0.0435	0.05271
1–0 $O(3)$	2.803	0.6108	1.164
1–0 $Q(1)$	2.407	0.6200	1.181
1–0 $Q(2)$	2.413	0.3001	0.6523
1–0 $Q(3)$	2.424	0.6196	0.9985
1–0 $Q(4)$	2.437	0.2167	0.3423
1–0 $Q(5)$	2.455	0.4508	0.4936
1–0 $S(0)$	2.223	0.2502	0.5436
1–0 $S(1)$	2.122	0.7724	1.245
1–0 $S(2)$	2.034	0.3254	0.5142
1–0 $S(3)$	1.958	0.7448	0.8152
1–0 $S(4)$	1.892	0.1946	0.1648
1–0 $S(5)$	1.836	0.4296	0.2585
2–1 $O(3)$	2.974	0.3380	0.6760
2–1 $Q(1)$	2.551	0.3365	0.6730
2–1 $Q(2)$	2.559	0.1688	0.3797
2–1 $S(0)$	2.356	0.1384	0.3112
2–1 $S(1)$	2.248	0.4132	0.6891
2–1 $S(3)$	2.074	0.3870	0.4286
3–0 $S(1)$	0.815	0.0149	0.0257

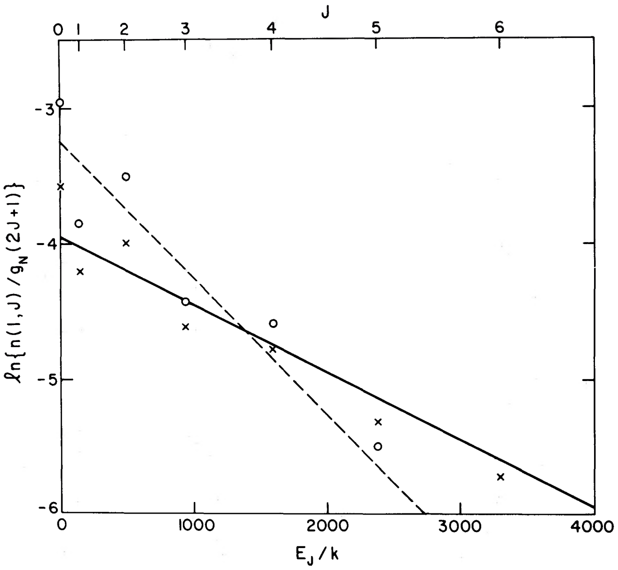

FIG. 1.—Populations of levels $v = 1$, J are shown as functions of the excitation energies, for associative detachment plus ultraviolet pumping at $T = 5000$ K (×) and $T = 1000$ K (○). The solid and dashed lines represent thermal populations at $T = 2000$ K and $T = 1000$ K respectively.

$A(vJ) = \sum_{v'' \leq v} A(vJ, v''J'')$ is the inverse lifetime of level (vJ). The emissivity in a transition $(v', J') \rightarrow (v'', J'')$ is now

$$j(v'J';\, v''J'') = n(v'J')A(v'J';\, v''J'') = n(\mathrm{H})n(\mathrm{H}^-)k\epsilon(v'J';\, v''J'') , \quad (16)$$

and values of the relative emissivities $\epsilon(v'J';\, v''J'')$ for selected transitions at $T = 5000$ K and $T = 1000$ K are listed in Table 5. Comparison of Table 5 with Tables 1 and 2 shows that the strengths of the high-J transitions are little affected by ultraviolet pumping while the transitions between levels of low J are greatly enhanced. In particular, ultraviolet pumping increases the emissivity in the 1–0 $S(1)$ line by a factor of 56. Even so, ultraviolet pumping can account for the relative strengths of the H_2 1–0 $S(1)$ and H Brackett lines in NGC 7027 only if the transition zone is thick, of the order $\delta r/r_0 \approx 0.1$. Such a large transition zone is unphysical in a dense nebula like NGC 7027.

In Figure 1, we present values of ln $[n(1, J)/g_N(2J + 1)]$ as a function of the excitation energies E_J for $T = 1000$ K and 5000 K, where $g_N = 1$ and 3 for even J and odd J respectively. The slopes of the lines through the points provide values of excitation temperatures. For the low J levels of $v = 1$, the populations at $T = 5000$ K are reproduced approximately by temperatures between 1500 K and 2000 K, and the populations at $T = 1000$ K are reproduced approximately by temperatures between 1000 K and 1400 K. The intensity ratios of lines within the fundamental band ($v = 1 \rightarrow 0$) must be measured with high precision in order to distinguish a spectrum due to associative detachment and radiative pumping from one due to thermal collisional excitation. As will be shown below, the intensity ratio of $v = 2 \rightarrow 1$ and $v = 1 \rightarrow 0$ lines discriminates sensitively between these excitation mechanisms.

c) *Collisional Excitations*

The kinetic temperatures $T = 1000$ K and 5000 K are high enough that electron-impact excitation of $v = 1$ and $v = 2$ may contribute to the line strengths. We estimated the excitation rates for the $v = 0 \rightarrow 1$ and $v = 0 \rightarrow 2$ transitions from the cross sections of Crompton, Gibson, and Robertson (1970), Henry (1970), Blevin, Fletcher, and Hunter (1978), and Klonover and Kaldor (1979). We assumed the rates to the individual rotational levels of the $v = 1$ and 2 states to scale according to the statistical weights. The calculated H_2 emissivities, including the effects of electron collisions upon the populations of levels of $v = 1$ and $v = 2$, are now sensitive to the competition between collisions and radiative excitation, a competition which may be characterized by the parameter ϕ/n, where ϕ is the flux of pumping photons at 1000 Å in photons cm^{-2} s^{-1} Hz^{-1}.

The abundances of H^- and of $H_2(v, J)$ were computed for the radiation field described in § II*b* with the assumption that $n(\mathrm{H}^+) = n(\mathrm{H}) \approx n(e)$. Photodetachment of H^-, equation (7), was included explicitly. The resulting emissivities of selected transitions at $T = 5000$ K and $T = 1000$ K are shown in Table 6 for several values of ϕ/n.

As ϕ/n decreases, collisional excitation processes increase the emissivities of lines of the 1–0 band including the high-J rotational transitions though their enhance-

TABLE 6

H_2 EMISSIVITIES INCLUDING COLLISIONAL EXCITATION OF THE $v = 1, 2$ VIBRATIONAL LEVELS EXCLUDING PURE ROTATIONAL TRANSITIONS IN THE $v = 0$ LEVEL

	$T = 5000$			$T = 1000$		
TRANSITION	$\phi/n = 10^{-10}$	$\phi/n = 10^{-9}$	$\phi/n = 10^{-8}$	$\phi/n = 10^{-13}$	$\phi/n = 10^{-12}$	$\phi/n = 10^{-10}$
1–1 $S(13)$	0.2882	0.1435	0.1307	0.0871	0.0687	0.0667
1–1 $S(11)$	0.8173	0.2046	0.1464	0.1580	0.0845	0.0763
2–2 $S(15)$	0.1041	0.1042	0.1046	0.0752	0.0752	0.0752
3–3 $S(15)$	0.0435	0.0436	0.0439	0.0527	0.0527	0.0527
1–0 $Q(1)$	24.16	3.000	0.9213	41.66	5.229	1.218
1–0 $Q(2)$	8.131	1.087	0.3970	7.904	1.377	0.6547
1–0 $Q(3)$	22.28	2.782	0.8570	18.12	2.711	1.013
1–0 $S(1)$	27.78	3.469	1.069	22.59	3.381	1.263
1–0 $S(2)$	10.15	1.301	0.4230	3.806	0.8434	0.5151
1–0 $S(3)$	32.07	3.846	1.023	10.25	1.760	0.8245
2–1 $Q(1)$	5.009	0.8124	0.4173	0.7832	0.6840	0.6706
2–1 $S(1)$	5.404	0.9129	0.4824	0.7445	0.6945	0.6873
2–1 $S(3)$	6.051	0.9470	0.4344	0.4513	0.4307	0.4283
3–0 $S(1)$	0.0149	0.0150	0.0158	0.0257	0.0257	0.0256
TOTAL	415.7	73.03	38.34	261.5	67.15	45.64

ment is small. The high-J rotational transitions in $v = 2$ and $v = 3$ are largely unaffected by either collisions or radiative excitation and they provide an unambiguous diagnostic probe of the associative detachment process.

III. DISCUSSION

Line emissions of H_2 have been detected in several regions of the interstellar gas (see Gautier *et al.* 1976; Treffers *et al.* 1976; Beckwith, Persson, and Gatley 1978; Beckwith *et al.* 1978*a*; Beckwith *et al.* 1978*b*; Simon *et al.* 1979; Ogden *et al.* 1979; Nadeau and Geballe 1979; Treffers 1979; Beck, Lacy, and Geballe 1979; Fischer, Righini-Cohen, and Simon 1980; Fischer *et al.* 1980; Knacke and Young 1980), and the excitation has been attributed to shock fronts passing through neutral material (see Kwan 1977; Hollenbach and Shull 1977; London, McCray, and Chu 1977). A shock front near to the boundary of a planetary nebula is close enough to the parent star that its H_2 vibrational population is modified by ultraviolet pumping. The emissivity is sensitive to the parameter ϕ/n, and the measurements of the ratio of the intensities of the $S(1)$ lines of the 1–0 and 2–1 bands can be used to constrain the value of ϕ/n in NGC 7027.

We adopt a kinetic temperature for the shocked gas of 1000 K (see Smith, Larson, and Fink 1981). Collisional excitation is dominated by neutral atom impacts, and our calculations show that $\phi/n < 10^{-13}$ if the lower limit of 5.6 observed for the intensity ratio is to be satisfied. For NGC 7027, observations have established that the electron density decreases outward from the central star to the outer boundary and that the mean value for a fully filled nebula is between 2×10^4 cm^{-3} and 6×10^4 cm^{-3} (Scott 1973; Harris and Scott 1976; Kaler, Aller, and Czyzak 1976; Atherton *et al.* 1979). Near the boundary, an electron density of 6×10^4 cm^{-3} is a plausible estimate. The corresponding density of neutral, shocked gas at $T = 1000$ K will be of the order of 6×10^5 cm^{-3}.

The flux ϕ_0 at 1000 Å, corresponding to the size of the nebula and the probable effective temperature of its exciting star (Miller and Mathews 1972; Atherton *et al.* 1979; Péquignot, Aldrovandi, and Stasinska 1978), incident on the outer boundary would be $\phi_0 = 10^{-4}$ photons cm^{-2} s^{-1} Hz^{-1} if unattenuated. Our limit on $\phi/n = \phi_0 \exp(-\tau)/n$ then implies an attenuation factor $\exp(-\tau)$ of at least 6×10^{-4} at 1000 Å because of internal extinction corresponding in the visual to an extinction A_v by dust of 1.5. The derived attenuation factor cannot be attributed to a zone of optically thick, self-shielded H_2 because the inner shell of such a zone would be the source of intense, radiatively-excited infrared emission lines.

A visual extinction A_v exceeding 1.5 is consistent with infrared and with visual observations (see Seaton 1979). Maps at high angular resolution show that the relative extinction varies by two magnitudes over the face of the nebula (Atherton *et al.* 1979), suggesting that much of the extinction occurs in the immediate vicinity of the nebula and is internal.

Although a neutral shock model is consistent with the observations, an alternative interpretation, not involving a shock, is also possible; this model incorporates vibrational population by formation and pumping in an internally shielded, ionized nebula. In the transition zone, electrons are more efficient than neutral atoms in producing excitation, and the upper limit of ϕ/n deduced from the intensity ratio of the $S(1)$ lines is increased to 10^{-12} if $T = 1000$ K and to 10^{-10} if $T = 5000$ K. For $n_e = 6 \times 10^4$ cm^{-3} at 5000 K, the limit can be satisfied by an internal extinction A_v exceeding 0.6.

Consider now a nebula with a transition zone of thickness 3×10^{14} cm with a column density $n\delta r$ of the order of 10^{19} cm^{-2}, half of which is neutral gas. The

TABLE 7

LINE INTENSITIES IN NGC 7027

	I	
Line	Observed[a]	Model
H Brγ	52.7	52.7
H_2 1-0 $S(1)$	3.7 ± 1.0	3.86
H_2 1-0 $Q(5)$	< 5	2.33
H_2 1-0 $Q(4)$	$\lesssim$ 1.3 ± 1.2	0.817
H_2 1-0 $Q(3)$	2.4 ± 1.0	2.71
H_2 1-0 $Q(2)$	1.2 ± 1.0	0.992
H_2 1-0 $Q(1)$	3.5 ± 1.1	2.96
H_2 2-1 $S(1)$	< 0.9	0.708
H_2 1-0 $S(0)$	1.0 ± 0.8	0.898
H_2 2-1 $S(2)$	< 0.8	0.270
H_2 2-1 $S(3)$	< 0.5	0.859
H_2 1-0 $S(2)$	0.9 ± 0.5	1.47
H_2 3-0 $S(1)$	< 0.6	0.0054

[a] The units are 10^{-12} ergs cm^{-2} s^{-1}, and the observed intensities are from Smith, Larson, and Fink (1981), except for the upper limit to the 3-0 $S(1)$ line which is from Traub, Carleton, and Black (1978).

nebula has a radius of 1.5×10^{17} cm, and the temperature is 10^4 K in the fully ionized region and 5000 K in the transition zone. The radiation field is such that $\phi/n = 10^{-10}$. Because of the high effective temperature of the central star and radiation hardening at the boundary, the ionizing photons typically have energies between 3 and 5 times the hydrogen ionizing threshold, and the cross sections are 30–100 times smaller than the threshold cross section. Thus the thickness of the transition zone is comparable to the photon mean free path. The volume density and the column density of H_2 are respectively 7 cm^{-3} and 2×10^{15} cm^{-2}. The optical depth at the center of any of the absorption lines of H_2 is unity or less, and self-shielding may be ignored.

The model nebula reproduces the intensity of the H Brγ line measured for NGC 7027. The calculated H_2 line strengths are listed in Table 7. With the exception of the $2 \rightarrow 1$ $S(3)$ line, they agree closely with the measured intensities. The discrepancy could be removed by a change in the extinction. The predicted intensity of the $3 \rightarrow 0$ $S(1)$ line at λ8150 is well below the measured upper limit of Traub, Carleton, and Black (1978).

The attenuation factor for internal extinction implies that a large fraction of the ionizing flux is absorbed by the grains. The observed infrared luminosity of NGC 7027 apparently requires a competition between the grains and the gas in absorbing the ionizing photons (Becklin, Neugebauer, and Wynn-Williams 1973).

Additional observations are needed to distinguish between the shock model and ultraviolet pumping of a quiescent zone. Figure 1 indicates that line ratios must be measured to high precision if departures from thermal equilibrium are to be identified correctly.

The lines which are specific evidence for the associative detachment process appear to be too weak to be detectable in planetary nebulae with available techniques. It may be more productive to search for the strongest lines in other partly ionized plasmas such as circumstellar shells of low density.

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