L(α)-INDUCED, TWO-PHOTON ABSORPTION OF VISIBLE LIGHT EMITTED FROM AN O-TYPE STAR BY H_2^+ IONS LOCATED NEAR THE SURFACE OF THE STRÖMGREN SPHERE SURROUNDING THE STAR: A POSSIBLE EXPLANATION FOR THE DIFFUSE INTERSTELLAR ABSORPTION BANDS (DIBS)

James H. Glownia and Peter P. Sorokin,
IBM Research Division,
T.J. Watson Research Center,
Yorktown Heights, NY 10598-0218

1. Introduction

The long-standing mystery in astronomy concerning the origin of the diffuse interstellar absorption bands (DIBs) was recently conveyed to *Physics Today* readers in an article (Huffmann, 1991) primarily concerned with describing the new field of fullerene research. Figure 1 (adapted from the above article) depicts the measured spectral dependence of the extinction that is generally attributed to interstellar dust. In Fig. 1a the optical density over a large energy range is shown. A smoothly varying main component is seen generally to increase with photon energy - displaying, however, an enormous "bump" at $\lambda \simeq 2175\text{Å}$ (5.7 eV). The diffuse interstellar bands appear as fine structure in Fig. 1a between about 1.9 and 2.8 eV. The DIB intensities generally correlate with the smoothly varying component of extinction ("reddening") seen in a given direction. In Fig. 1b, the appearance of DIBs with the smoothly varying extinction component subtracted is depicted.

A convincing explanation of the origin of the DIBs has evidently thus far not materialized. They are generally believed to be of interstellar origin - hence, the term: diffuse *interstellar* bands. Most recent explanations are solid-state based. Many postulate the existence in interstellar space of large organic molecules, such as polycyclic aromatic hydrocarbons (PAHs), long chain unsaturated hydrocarbons, fullerenes, etc., perhaps adsorbed onto various (unspecified) dust particles. With such models, serious difficulty is encountered in trying to account for the seemingly universal presence in interstellar space of the large and complex molecular structures whose existence is postulated. Furthermore, spectra predicted by the various models proposed thus far do not come very close to matching the fascinating and intricate spectral signature presented by the DIBs.

In this paper, a new model is proposed to account for the DIBs. In this model, the DIBs result from a *non-linear* effect: resonantly-enhanced two-photon absorption of H_2^+ ions located near the surface of the Strömgren sphere that surrounds an O- or B-type star. The strong light (at ω_1) that is required to "drive" the two-photon transition is provided by L(α) light emerging from the Strömgren sphere that bounds the H II region surrounding the star. In Sec. 2, a value $\simeq 200$ μW/cm² is estimated for the L(α) flux at the Strömgren radius, R_s, of a strong (O5) star. (A pure hydrogen star is assumed.) It is shown in Sec. 3 that a c.w. L(α) flux of this intensity should be sufficient to induce a few percent absorption for visible light radiated by the same

star at a frequency (ω_2) that completes an allowed two-photon transition, provided (1) the L(α) radiation happens to be nearly resonant with the frequency of a fully-allowed absorber transition that effectively represents the first step in the two-photon transition, and (2) an effective column density $\sim 10^{18}/cm^2$ of the absorber is present near the Strömgren sphere radius, R_S. In Sec. 4, it is shown that a few *almost exact* resonances (i.e., with frequency offsets from L(α), Δ, not exceeding $\simeq 2$ cm^{-1}) are found in the allowed H_2^+ system: $2p\pi_u(v', J') \leftarrow 1s\sigma_g$ (v", J"). It is then indicated that the "second step" H_2^+ transitions: [$4d\sigma_g$, $5g\sigma_g$, $3d\delta_g$, $5g\pi_g$, $4d\pi_g$, and $3s\sigma_g$] $\leftarrow 2p\pi_u$ (v', J') can possibly account for the DIBs. This visible absorption spectrum is, in principle, exactly calculable. To begin to explore whether or not there might really exist exact coincidences between measured locations of DIBs and transition wavelengths predicted by the model, one could initially attempt to compute vib-rot level energies for the (four) above even-parity states that are bound, preferably with adiabatic corrections incorporated into the Born-Oppenheimer approximation.

The required presence of H_2^+ molecules located near R_s could conceivably result from direct photoionization of H_2 molecules located in a compact shell that serves as the transition region between the H II sphere and the cold surrounding hydrogen gas. In this case, one would expect the H_2^+ ions to be produced in the ground state with a vibrational distribution given by the known Franck-Condon factors for ionization of hydrogen. It is, therefore, quite interesting that the *linear* H_2^+ absorption spectrum one calculates for such a distribution has generally similar features to those possessed by the smoothly-varying component of the measured "interstellar" extinction curve, including the large "bump" at $\simeq 2175$ Å.

2. L(α) radiation emerging from radiatively excited nebulae of pure hydrogen (H II regions)

The source of excitation of the gas is assumed to be an embedded bright star of early spectral type - for example, an O- or a B-type star. We rely here on the simplest model for this gas - as described, for example, in Chapter 5 of the text by Dyson and Williams (Dyson and Williams, 1980). Table 1, adapted from Table 5.3 of one of Spitzer's books (Spitzer, 1978), shows what the total rate of photon emission shortward of the Lyman limit for typical O and B stars is. We here assume that our embedded star is like the O5 one listed, with $N_u \simeq 5 \times 10^{49}$ s^{-1}. Note that the radius of the star is only 13.8 x $R_\odot$, or 3.2 x 10^{-7} parsec (pc).

Spectral Type	T_{eff}(°K)	$R/R_\odot$	$N_u(s^{-1})$
O5	47,000	13.8	51 x 10^{48}
O6	42,000	11.5	17.4
O7	38,500	9.6	7.2
O8	36,500	8.5	3.9
O9	34,500	7.9	2.1
B0	30,900	7.6	0.43
B1	22,600	6.2	0.0033

Table 1. Radiative Properties of Early-Sequence Stars

Let us estimate the L(α) flux emerging from the "Strömgren sphere" (the sphere whose radius, R_s, delineates the boundary between the almost fully ionized H II interior, and the cold hydrogen gas exterior). We have, approximately,

$$4\pi R_S^2 \Psi_{L(\alpha)} = \frac{4}{3}\pi R_S^3 n_e^2 \beta_2(T_e) \tag{1}$$

This equation assumes that there is one L(α) photon produced for every recombination (to n$\geq$2) that occurs. Also, if a L(α) photon is absorbed by an H atom, it will simply be re-scattered in another direction. All L(α) photons produced will eventually escape through the surface of the Strömgren sphere.

An excellent numerical approximation for the total recombination coefficient, $\beta_2(T_e)$, is (Dyson and Williams, 1980):

$$\beta_2(T_e) = 2\times10^{-16}T_e^{-3/4}m^3 s^{-1}, \tag{2}$$

where T_e is the temperature of the gas in the H II region. Estimates of such temperatures lie roughly in the range 5,000 - 10,000 K, with rather little variation from one nebula to the other (Dyson and Williams, 1980). We assume T_e = 10,000 K for our case. Then $\beta_2 \simeq 2 \times 10^{-19}$ m^3 s^{-1}.

The Strömgren radius, R_s, is given by (Dyson and Williams, 1980):

$$R_S = \left(\frac{3N_u}{4\pi n_e^2 \beta_2}\right)^{1/3} m. \tag{3}$$

Thus, combining this with Eq(1), one has:

$$\Psi_{L(\alpha)} = \frac{1}{3}n_e^{4/3}\beta_2^{2/3}\left(3\frac{N_u}{4\pi}\right)^{\frac{1}{3}}. \tag{4}$$

Let's assume that n_e = 10^5 cm^{-3}. Then one has: $\Psi_{L(\alpha)}$ = 1.21 x 10^{18} photon s^{-1} m^{-2}. This is a L(α) intensity of about 200 μW/cm^2.

For the parameters chosen, the value of R_s is about 1.8 x 10^{15} m, or about 0.06 pc. - some 2 x 10^5 times greater than the radius of the embedded O5 star. If one multiplies 4π times the square of R_s times the L(α) flux calculated above, one gets back, of course, 5 x 10^{49} photons s^{-1}.

From the discussion given above, the linewidth of the L(α) radiation emerging from an H II region has to be the Doppler width at the temperature T_e. This is given by the formulas (Spitzer, 1978):

$$\Delta v = \frac{2(\ln 2)^{1/2}b}{\lambda}, \tag{5}$$

with

$$b = 1.290\times10^4\left(\frac{T_e}{A}\right)^{1/2} cm/\sec. \tag{6}$$

Choosing T_e to be 10,000K, A (atomic weight) to be 1, and λ to be 0.1215 x 10^{-4} cm gives Δv $\simeq$6 cm^{-1}. Observed DIB linewidths can be both larger and smaller than the L(α) linewidth assumed in our model.

3. Resonant enhancement of two-photon absorption cross-section

For linearly polarized light waves, the absorption cross-section of an atom (or molecule) for light at frequency v_2 induced by light at v_1 for transitions from the ground state g to the excited state f is given by (Bjorkholm and Liao, 1974):

$$\sigma(v_2) = 1.15\text{x}10^{-34} \, | \sum_n <f|z|n><n|z|g> [(E_n - hv_2)^{-1} + (E_n - hv_1)^{-1}] |^2 \, v_2\rho(v_2 + v_1)I_1 \quad cm^2, \quad (7)$$

where I_1 is the intensity in W/cm^2 of the radiation field at v_1, $\rho(v_2 + v_1)$ is the normalized lineshape function for the (H_2^+) transition, the matrix elements are expressed in Bohr radii, and the summation is carried out over all intermediate states of energy E_n, expressed in rydbergs. For the 3s-4d transitions in Na (with the 3p levels as the dominant intermediate states), use of Eq. (7) leads to the result (Bjorkholm and Liao, 1974) that the induced cross-section for this transition is approximately (5 x 10^{-16}) I_1 cm^2 when E_{3p} - hv_1 = 1.0 cm^{-1}. With an effective detuning of 1.0 cm^{-1} and with I_1 = 200 μW/cm^2, a column of (for example, H_2^+) ground state molecules of length 10^{16} cm (0.003 pc) and of density 100/cm^3 could thus, in principle, absorb 10% of the visible background light at those frequencies completing two-photon resonances. Note that the total H_2^+ column length (0.003 pc) needed here is only about 5% of the Strömgren radius (0.06 pc) in this case.

4. H_2^+ transitions that are nearly resonant with L(α) and those that complete the two-photon absorption process

If a vibrational level v'' of the 1sσ_g ground electronic state has a good Franck-Condon overlap with a vibrational level v' of the 2pπ_u excited state, transitions between the two levels are strongly allowed. Using adiabatically corrected values (Bishop et al., 1975) for the vib-rot levels of these two electronic states, one can show that the P(1) line of v'=5 $\leftarrow$ v''=15 almost exactly coincides with the *peak* wavelength of the L(α) radiation, and that the P(1), Q(2), and R(3) lines of v'=11 $\leftarrow$ v''=18 are all within 2 cm^{-1} of the L(α) peak. *The DIB wavelengths in the model proposed here should thus correspond to wavelengths of allowed transitions from (low J' value) 2pπ_u states with v'=5 and v'=18 to even-parity states dissociating to H$^+$ + H(n$\geq$3)*. Although Born-Oppenheimer potentials for the twelve states dissociating to H$^+$ + H(n=3) have been calculated (Madsen and Peek, 1971), vib-rot level energies for the (bound) states have not, for example, been determined. Hence, until accurate calculations for these states become available, the best procedure for estimating DIB wavelengths from the model is to determine vertical energy separations between upper and lower potential curves at the *right-hand turning points of v'=5 and v'=11*, i.e., at 13.0 a_o and at 20.5 a_o (Fig. 3). We illustrate by carrying out this procedure for the 3dδ_g $\leftarrow$ 2pπ_u transition. This has a large, constant (i.e., as a function of R) dipole moment of 3.00 a.u. (Ramaker and Peek, 1972). A vertical line drawn at 20.5 a_o intersects the 3dδ_g potential curve at a point $\simeq$282 cm^{-1} below its dissociation energy. The upper level for this transition is thus stable and would not contribute to the DIB linewidth, which would in this case presumably be primarily determined by the spectral extent over which resonance enhancement given by Eq. (7) occurs. The predicted DIB wavelength is

here 6679 Å. Could this possibly be the strong, narrow (width at half depth $\simeq$ 2.5 cm^{-1}) DIB observed at 6614 Å? At 13.0 a_o, a vertical line intersects the $3d\delta_g$ potential at a point $\simeq$178 cm^{-1} *above* its dissociation energy (and 125 cm^{-1} above the height of the shallow "barrier" existing at R = 37.5 a_o). The DIB transition, predicted in this case to occur at 6156 Å, should thus be strongly broadened. Could this be the strongly broadened DIB (width at half depth $\simeq$ 80 cm^{-1}) that is observed at 6177 Å? In Table 2, we show the wavelengths that are generated in carrying out this procedure for all six even-parity states dissociating to H^+ + $H(n=3)$. Wavelengths predicted to be sharp (s) or diffuse (d) are so indicated.

Upper State	R = 13.0 a_o	R = 20.5 a_o
$5g\pi_g$	4054 Å (d)	5959 Å (d)
$4d\pi_g$	4658 Å (d)	5749 Å (d)
$3d\delta_g$	6156 Å (d)	6679 Å (s)
$5g\sigma_g$	4669 Å (d)	9219 Å (s)
$4d\sigma_g$	6215 Å (s)	6842 Å (s)
$3s\sigma_g$	4467 Å (d)	5441 Å (d)

Table 2. Predicted DIB Wavelengths

5. Is H_2^+ possibly also the source of the "bump" at $\lambda \simeq$ 2175 Å?

As stated in the Introduction, the required presence of H_2^+ molecules located near R_s could conceivably result from direct photoionization of H_2 molecules in a compact shell that serves as the transition region between the H II sphere and the cold surrounding (H_2) gas. In this case, one would expect the H_2^+ ions to be produced in the ground state with a vibrational distribution given by the known Franck-Condon factors for ionization of hydrogen. It is apparent from the Dunn and Oksjuk results (Fig. 4) that the cross-section for $2p\sigma_u \leftarrow 1s\sigma_g$ photodissociation for such a vibrational distribution peaks somewhere in the 2100 - 2200 Å range. Thus, an intriguing additional feature appears in the model presented here!

One can even "push one's luck" and try to ask why the interstellar extinction curve reverses its decline at $\simeq$8 eV, after it has fallen considerably from its 2175 Å peak, and strongly starts to increase again with increasing photon energy. A possible explanation is that at shorter wavelengths the vibrational H_2^+ $1s\sigma_g$ distribution that results from H_2 photoionization starts to absorb again when the photon energy becomes high enough for the $2p\pi_u \leftarrow 1s\sigma_g$ transition to occur. There are also allowed transitions from $1s\sigma_g$ to higher states of u parity, states dissociating both to n=2 and higher n.

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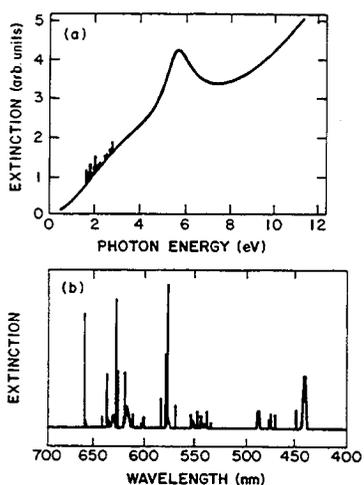
Fig. 1. Extinction due to interstellar dust (Huffman, 1991).

Fig. 2. Some potential curves for H_2^+ (Levine, 1974).

Fig. 3. $1s\sigma_g$ and $2p\pi_u$ potential curves (Beckel, C.L.; Shafi, M.; and Peek, J.M.: 1973, J. Chem. Phys. **59**, 5288).
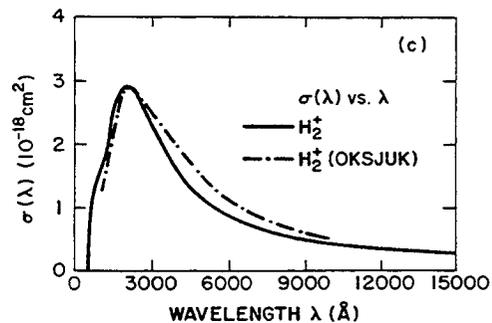
Fig. 4. $\sigma(\lambda)$ [$2p\sigma_u \leftarrow 1s\sigma_g$ transition] for the H_2^+ vibrational distribution produced by photoionization of H_2 (Dunn, 1968).