

Molecular Hydrogen Optical Depth Templates for *FUSE* Data Analysis

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ABSTRACT

The calculation and use of molecular hydrogen optical depth templates to quickly identify and model molecular hydrogen absorption features longward of the Lyman edge at 912 Å are described. Such features are commonly encountered in spectra obtained by the Far Ultraviolet Spectroscopic Explorer and also in spectra obtained by the Space Telescope Imaging Spectrograph, albeit less commonly. Individual templates are calculated containing all the Lyman and Werner transitions originating from a single rotational state (J'') of the 0th vibrational level (v'') of the ground electronic state. Templates are provided with 0.01 Å sampling for doppler parameters ranging from $2 \leq b \leq 20$ km s⁻¹ and rotational states $0 \leq J'' \leq 15$. Optical depth templates for excited vibrational states are also available for select doppler parameters. Each template is calculated for a fiducial column density of $\log[N(\text{cm}^{-2})] = 21$ and may be scaled to any column less than this value without loss of accuracy. These templates will facilitate the determination of the distribution of molecular hydrogen column density as a function of rotational level. The use of these templates will free the user from the computationally intensive task of calculating profiles for a large number of lines and allow concentration on line profile or curve-of-growth fitting to determine column densities and doppler parameters. The templates may be downloaded freely from the URL <http://www.pha.jhu.edu/~stephan/h2ools2.html>.

Subject headings: ISM: abundances – ISM: molecules – line: identification – line: profiles – methods: analytical – molecular data – ultraviolet: ISM

1. Introduction

The launch of the Far Ultraviolet Spectroscopic Explorer *FUSE* has opened a new spectral window on the universe with a 905 – 1187 Å bandpass (Sahnow et al. 2000). Within this window spectra of continuum emitting objects almost universally exhibit absorption bands of molecular hydrogen, indicating this gas resides in the interstellar medium somewhere between the object and the observer. These bands arise from the photo-excitation of molecular hydrogen by the background continuum object, causing electrons in the

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ground electronic state $X^1\Sigma_g^+$, to be excited into either the higher $B^1\Sigma_u^+$ (Lyman band), or $C^1\Pi_u$ (Werner band) states. The strength and density of the absorption lines are proportional to the distribution of molecular hydrogen column densities among the ground state rotational and vibrational (J'' , v'') energy levels² peculiar to the line-of-sight.

For some observers the molecular hydrogen electron population distribution within the ro-vibrational states is a subject of direct interest. For others, molecular hydrogen absorption is a nuisance, potentially contaminating or even obscuring spectral features of interest. Fortunately there is a high degree of correlation between the absorption lines within different ro-vibrational bands ($v' - 0$) imposed by the uniformity of the energy level separations and the slow monotonic variation of oscillator strength as a function of upper vibrational state, a consequence of the Franck-Condon principle (Herzberg 1950). This correlation greatly aids the identification of molecular hydrogen features and provides a means for their removal from blended features, provided they can be reliably modeled in an unobscured portion of the spectrum.

Here we will discuss the calculation and use of a simple set of optical depth templates from which observers can easily identify and model the molecular hydrogen features commonly observed in the *FUSE* spectral range. Each template contains all the Lyman and Werner absorption lines arising from the photo-excitation of electrons out of common ground state rotational J'' and vibrational $v'' = 0$ levels (usually) and into the v' states of the upper bands ($v' \leftarrow 0$), subject to the appropriate rotational state selection rules. A single column density $N(v'', J'')$ controls the line strength and the templates are scaleable with this quantity. The optical depth variation with wavelength for each line is calculated using a Voigt profile to allow for the proper variation of line shape with increasing column density, reproducing the shapes endemic to the linear, flat, and square root portions of the curve-of-growth as controlled through the specification of the doppler parameter (b). The templates are given as optical depths functions, as opposed to transmission functions, to facilitate the inclusion of various atomic and molecular species or multiple velocity structures, simply by adding additional optical depths to the template function at the appropriate wavelength position.

These templates can be used in conjunction with a variety of methods to determine the appropriate column densities and doppler parameters. One method is direct profile fitting, where the templates for various $N(v'', J'')$ and b are used with a predetermined continuum to directly compare to the observed spectrum in a χ^2 calculation. Another method uses the curve-of-growth technique, where equivalent width measurements are used to determine the appropriate column and doppler parameter from which the absorption line transmission function can be quickly calculated. Once the columns, doppler parameters and continua are known in an unblended portion of the spectrum the degree to which they effect the other features, such as O VI or D I, maybe assessed.

The template calculations incorporate the Abgrall et al. (1993a,b) databases of transition lifetimes, wave-numbers, rotational and vibrational quantum numbers for Lyman and Werner band transitions. The templates are available for free access on-line through <http://www.pha.jhu.edu/~stephan/h2ools2.html>.

²When referring to the rotational and vibrational quantum numbers in a transition going from an upper electronic state (e.g. either $B^1\Sigma_u^+$ or $C^1\Pi_u$) to the ground state ($X^1\Sigma_g^+$) it is traditional to designate the upper state numbers with a single prime (e.g. J' , v') and the lower state with a double prime (e.g. J'' , v'').

Here we provide potential users with a ready reference to the calculation procedures, some examples of use, and discuss appropriate positional accuracy and column density limitations. We include formulae for the calculation of energy levels, population distributions, and line profiles in Appendices A and B.

2. Energy Levels, Population Distribution, and Selection Rules

The ground state rotational energy levels in the $v'' = 0$ vibrational state have temperature equivalent energies $B_v hc/k \approx 0, 170, 510, 1014, 1680, 2500$ K for $J = 0 \rightarrow 5$, while the vibrational energy levels are much more widely spaced with separations $\Delta G'' hc/k \equiv (G(v'' + 1) - G(v''))(hc/k) \lesssim 5983$ K (see Appendix A). Boltzmann's law shows that the first few rotational states are low enough to be populated at the relatively cold temperatures associated with molecular gas in the interstellar medium, while excitation of the upper vibrational levels requires a more energetic environment. Absorption from several rotational levels is the norm, although the early *Copernicus* observations showed the typical distribution of column density in the higher rotational states is larger than expected from a single temperature Boltzmann distribution (Aannestad & Field 1973). The reasons for the deviations from a Boltzmann distribution are myriad and we refer to the reader to the comprehensive review by Shull & Beckwith (1982) who have discussed the various diagnostics for determining formation rates, collision rates and local radiation field intensity by using the rotational column density distribution of molecular hydrogen and the atomic hydrogen column. Absorption from excited vibrational states are rare. When present they indicate that the gas is affected by either a high temperature process such as shocks (McCandliss 2001) or a nonthermal processes such as fluorescent pumping (Meyer et al. 2001).

Lyman bands have two branches R(J''), with $J' = J'' + 1$ and P(J''), with $J' = J'' - 1$. The selection rule that requires $\Delta J = \pm 1$ results from the zero change in electronic angular momentum between the $X^1\Sigma_g^+$ and $B^1\Sigma_u^+$ states (Herzberg 1950). The Werner bands have an additional branch Q(J'') with $\Delta J = 0$, allowed because the change in electronic angular momentum between the $X^1\Sigma_g^+$ and $C^1\Pi_u$ states is one. In addition, the minimum J' for the $B^1\Sigma_u^+$ state is 0, while the minimum J' for the $C^1\Pi_u$ state is 1. This leads to an absence of P(0) in the Lyman bands and P(0), P(1) and Q(0) in the Werner bands.

There are 377 absorption line transitions from Lyman ($0 \leq v' \lesssim 20$) and Werner ($0 \leq v' \lesssim 5$) bands arising from rotational levels, $0 \leq J'' \leq 6$ in the ground vibrational level ($v'' = 0$) of the $X^1\Sigma_g^+$ electronic state longward of the Lyman edge. Many more are possible if $v'' > 0$ becomes populated. Consequently the identification of the molecular hydrogen lines can be daunting. It is typically the first task in the post pipeline analysis of *FUSE* spectra. The identification process is eased considerably by locating the strongest Lyman lines usually R(0) for $J'' = 0$ and P(1), R(1) for $J'' = 1$, and then proceeding to higher J'' until the lines merge with the noise. Our computation of templates containing only those lines originating from a single rotational state allows for a direct implementation of this method. It greatly facilitates the determination of the $N(v'', J'')$ distribution, and allows for assessing the degree of contamination in coincident alignments of molecular hydrogen absorptions with lines from other diagnostically useful atoms or molecules.

3. Optical Depth Template Calculation

A total optical depth function is constructed for the J'' rotational state of the $v'' \equiv 0$ vibrational level from the sum of all the individual optical depth profiles ranging over all v' states in the Lyman ($0 \leq v' \leq 18$) and Werner ($0 \leq v' \leq 5$) line database given as,

$$\tau_{J''}(\lambda) = \sum_{v'=0}^{v''_{max}} \tau_i(\lambda). \quad (1)$$

The function $\tau_{J''}(\lambda)$ is established on a common wavelength grid spanning the region of interest (790 – 1490 Å in our case) with 0.01 Å spacing. This total optical depth function is used to accumulate individual optical depth profiles. Each line profile is calculated using the Voigt function formulae in Appendix B, covering a range of wavelengths spanning 50 Å to either side of the line center, so as to accommodate the broad Lorentzian wings that appear in the line profiles at high column density. The span of the common wavelength grid is arbitrary. It allows for the convenient inclusion of contributions from lines of absorbing species both inside and outside of the *FUSE* bandpass. An insertion point is determined to be the wavelength grid point closest to the line center and the individual optical depth profile is added to the total optical depth about that point and the process is repeated for all Lyman and Werner transitions arising from the same lower level rotational state.

For the $J'' = 0$ states the template contains only the R(0) lines of the Lyman and Werner bands of ($v' \leftarrow 0$). For $J'' = 1$ there are R(1) and P(1) lines in the Lyman bands and R(1) and Q(1) lines in the Werner bands. Above $J'' = 1$ there are R(J'') and P(J'') lines in the Lyman bands and R(J''), Q(J'') and P(J'') lines in the Werner bands. A representative set of templates for $0 \leq J'' \leq 4$ with a doppler parameter of 5 km s⁻¹ with log columns of 21 and 20 for $J'' = 0, 1$, 19 to 18 for $J'' = 2$, 17 for $J'' = 3$, and 16 for $J'' = 4$. are displayed in Figure 1.

4. Line Position, Equivalent Width and Column Density Limits

The location of each line within the larger wavelength grid is accurate to within the grid step or 3 km s⁻¹. This method of insertion is computationally expedient compared to the more accurate but much slower method of interpolating the centered profile onto the 0.01 Å grid. Our grid spacing is on the order of the largest differences between observed and calculated wave-numbers in the Abgrall et al. (1993a,b) databases (~ 1 cm⁻¹). The resolution of the *FUSE* spectrograph is $R \approx 20000$ or 15 km s⁻¹ (Sahnou et al. 2000), so the grid oversamples by a factor of 5.

The minimum grid step of 0.01 Å sets a lower limit on the useful doppler parameter range. The core of a line with a doppler parameter of 1 km s⁻¹ is not sampled with sufficient resolution to yield an accurate measure of optical depth with increasing distance from the line core. Consequently, the numerically integrated equivalent width from the 1 km s⁻¹ template is higher than the theoretical value in the linear portion of the curve-of-growth and lower in the flat portion of the curve-of-growth. Although available on the website, the 1 km s⁻¹ templates should not be used for quantitative work. This problem is quantified in Figure 2 where we show curves-of-growth (in red) for a range of $Nf\lambda$, and a discrete set of doppler parameters ($b=1$,

2, 4, 8, and 16 km s⁻¹). Overplotted are the equivalent widths derived from direct numerical integration of the Lyman lines in the J=0 and J=1 templates over the same range of doppler parameters. The problem with the equivalent widths calculated from the lines contained in the b = 1 km s⁻¹ template is evident. There is a slight (< 7%) residual from the theoretical curves in b = 2 km s⁻¹ derived equivalent widths.

An examination of the current literature shows that very few lines-of-sight have been found with molecular hydrogen determined doppler parameters < 2 km s⁻¹. For example, in a study of the Large and Small Magellanic clouds Tumlinson et al. (2002) find only two lines-of-sight (out of 37 determinations) that have molecular hydrogen doppler velocities of < 2 km s⁻¹, although several have lower bounds that dip below b = 2 km s⁻¹. Another study by Meyer et al. (2001) finds a b = 1.8 (±0.1) km s⁻¹ for the highly excited molecular hydrogen in the line-of-sight toward HD 37903, the central star of the reflection nebula NGC 2023. These instances notwithstanding, the current set of templates should be adequate for most work. We note that lines-of-sight with b = 2 km s⁻¹ will have instrumental line profiles, except where column densities are high enough to produce damping wings. The curve-of-growth technique will be preferred to line profile fitting for determining column densities and doppler parameters in these instances, as noted in the following section. The templates are not used in the curve-of-growth analysis except to represent the solution after it has been found. The regime where absorption lines will have instrumental profiles in the FUSE spectrographs is roughly identified in Figure 2 as the region below the solid horizontal line drawn at log W/λ = 1/R.

Nevertheless there are many cases where small doppler velocities have been measured in species that correlate well with molecular hydrogen, as in the case of CH (e.g. Andersson, Wannier, & Crawford (2002) and Federman (1982)). In order to support such investigations in the future, templates will be developed with finer wavelength and doppler velocity grids for exploring the low b regime. Higher resolution grids will also find use in studies requiring closely spaced multiple velocity components with small doppler velocities. However, the current set of grids are large (≈ 8Mbyte uncompressed for a single b up to J'' = 15) and the high resolution grids will be at least twice as large.

The column densities have no lower limits, they may be scaled to as low a column as required without loss of accuracy. An upper limit results from the finite wavelength span of ±50 Å for the individual profile calculations. Above log N(v'', J'') = 21 (the fiducial column density for which each optical depth template is calculated) the individual line profiles suffer a progressively severe truncation of the Lorentz wings at ±50 Å from line center, which manifests itself as a series of discontinuities in the summed optical depth grid. The log N(v'', J'') ≲ 21 is a “fuzzy limit” as the seriousness of the truncation depends upon the oscillator strength. This effect is independent of doppler parameter because at log N(v'', J'') ≥ 21 all lines are fully damped for b < 20 km s⁻¹.

The effect is illustrated in Figure 3 with the lines of minimum and maximum oscillator strength in the R(0) transitions of the Lyman bands (0 – 0) and (7 – 0), where we show the half profiles of these two lines over a 50 Å span. We see that for a column density of log N(0,0) = 21 the line profile has returned from black at the line core to 0.9995 and 0.9990 at 50 Å from line center for (0 – 0) and (7 – 0), respectively. For a column density of log N(0,0) = 22 the lines only return to 0.995 and 0.990, while for log N(0,0) = 23

the return is 0.95 and 0.90, respectively. It is difficult to estimate quantitatively the combined effects of profile truncations since the error it generates is a function of wavelength. The general effect is to cause a progressive underestimation of the combined blackness of the rotational template for column densities $\log N(v'', J'') \geq 21$. Quantitative work at columns much greater than $\log N(v'', J'') \geq 21$ using these templates should be avoided. This should not be too much of a problem as few sight lines with $\log N(v'', J'') > 21$ have been found. For instance, in an exploration of 23 sight lines with $A_V \gtrsim 1$ Rachford et al. (2002) found only 1 case (HD 154368) where the formal value of $\log N(J'' = 0)$ was 21.04 ± 0.05 .

5. Discussion and Examples

The templates are stored in files with names that encode the calculation parameters. For example, tauh2n21b2j0-15v0.dat, indicates a column density of $\log N(\text{cm}^{-2}) = 21$, a doppler width of 2 km s^{-1} , a rotational state range of $0 \leq J'' \leq 15$, and a ground vibrational state of $v'' = 0$. The files contain 17 arrays of unformatted double precision numbers with 59000 elements. The first array is the wavelength variable. The next 16 arrays are the $J'' = 0, 1, \dots, 15$ optical depth functions. Table 2 gives a schematic of how the data arrays are placed in the file. A simple IDL program is provided on the website to read in the data and form an example transmission function. There are extra empty elements longward of the *FUSE* long wavelength cutoff at 1189 \AA in part because there are a few high rotational lines that exist beyond this cutoff. However, the main reason is to allow for the inclusion of spectra for ground state vibrational levels $v'' > 0$, for the purpose of investigating molecular hydrogen excitation processes in energetic astrophysical environments. Rotational templates for $v'' > 0$ states will be included on the H₂ools website in the near future.

Absorption spectra (the transmission functions) are obtained by taking e^{τ_λ} . All the optical depth templates are tabulated as negative numbers. The spectra for column densities other than 10^{21} particles cm^{-2} can be obtained by dividing the optical depth by 10^{21} and multiplying by the required column density value. For example, the absorption spectrum for 10^{18} is given by $e^{\tau_\lambda/1000}$. These spectra should be convolved with an instrumental line spread function to simulate instrumental broadening before comparing to an object spectrum. For use with *FUSE* spectra, convolution with a gaussian width with a FWHM on the order $R \gtrsim 15000$ is typical. For high precision work it may be necessary to employ a wavelength dependent convolution kernel, as the resolution of the various spectral channels is wavelength dependent at the 10% level (Sahnou et al. 2000).

Once convolved, an overlay of the $J'' = 0$ transmission function (multiplied by an appropriate continuum) on an object spectrum will allow an assessment of the need for zero-point offsets to the wavelength registration. The $J'' = 0$ spectrum contains the bluest lines in any given Lyman band ($v' - 0$), so it should line up with the blue side of the blended R(0) and R(1) lines. For the highly damped lines encountered at high column density it may be necessary to include higher J'' states to assess zero-point offsets. Adjust the column density of the absorption spectrum until a good fit is obtained. Once satisfied add the optical depth template from the next highest rotational state, take the exponent, adjust the columns and wavelength zero-point as necessary, and reassess the fit. Repeat until the inclusion of a higher level J'' no longer improves

the fit. The process may be quantified by computing the χ^2 statistic over wavelength intervals selected to coincide with unblended absorption features in the object spectrum. Repeat for different column densities and doppler parameters and then find the minimum χ^2 .

It is often expedient to perform the initial fitting operation by eye. Interactive assessment can be used to determine the columns to within a few dex and the doppler parameters within a few km s^{-1} , provided complicated velocity structures on the line of sight are absent and the column density is high enough. These approximate determinations can serve as the starting point for more precise work and minimize the time devoted to χ^2 minimization by providing good guesses. In Figure 4 we show how the higher vibrational transitions can be used to define the column and the lower vibrational transitions the doppler parameter when the absorptions are making the transition from the flat portion of the curve-of-growth to the square root portion where the lines profiles become fully damped. At $\log N(J'' = 0) = 19$ we see little difference in the higher vibrational line profiles for the two doppler parameters, while the lower vibrational lines do show a difference. At low doppler parameter the lines are still saturated, having box like profiles, while damping wings have developed in the higher doppler parameter line.

In the low column transition region ($\log N(J'' = 0) \sim 15$) between the linear and flat portion of the curve-of-growth, discerning the tradeoff in column and doppler parameter is less apparent to the eye. In this regime the lines are unresolved (by *FUSE*) and will have profiles close to the instrumental profile except for the highest doppler parameters. In these cases the curve-of-growth method for determination of column is generally more useful than profile fitting. In between these two regimes on the flat (slowly varying) portion of the curve-of-growth, it is relatively easy to determine the doppler parameter (b) from the box like profiles, but the column is ill-defined. Here profile fitting is the most accurate method for column determination.

In Figure 5 we show a curve-of-growth example. The molecular hydrogen column densities and a doppler parameter have been derived from a curve-of-growth analysis of all the lines in the rotational states $0 \leq J'' \leq 5$ between 1040 – 1098 Å. The bottom right panel for the (4–0) Lyman band fit shows an overplot of the transmission function computed by applying the derived column densities and doppler parameter. A curve-of-growth analysis was then applied to eight D I lines starting at Lyman- γ . An absorption line model containing lines from H I, D I, O I, and molecular hydrogen has been overplotted in each panel.

In Figure 6 we show an example of a χ^2 fit to the (4–0) Lyman band in the lower panel, which was fine-tuned by taking into account the fit to the (0–0) Lyman band. The rotational templates were used with an appropriate continuum to calculate χ^2 for selected portions of the line profiles. In the upper panel we illustrate how well the H₂ model from the (4–0) band fit reproduces the H₂ structures in the (5–0) band. The template model can be used to constrain the location and degree of blending with lines of O VI, C II, O I and Ar I. Several unidentified lines are also evident, some of which are higher rotational level H₂ lines.

These are just two examples illustrating how the use of these templates can expedite the identification, computation and deblending of molecular hydrogen profiles from far-UV spectra. The use of a common 0.01 Å wavelength grid facilitates the inclusion of profiles from other atomic and molecular species. In addition, any number of multiple velocity components can easily be coadded and scaled, with the appropriate doppler dilatation or contraction applied through the interpolation of the optical depth template onto a

shifted wavelength grid. Such interpolated optical depth templates can be employed to search for molecular hydrogen in intervening intergalactic absorption systems that appear in the spectra of quasars and galaxies at high redshift. The templates can find use in any study that requires an accounting for molecular hydrogen blending. Examples include studies seeking to determine the velocity distribution and abundance of O VI in the galaxy and halo, of D I in the local and nearby ISM, or of any other interstellar atomic and molecular species that may blend with molecular hydrogen features. The templates also provide a means to determine the excitation state of molecular hydrogen so as to directly test the predictions of various excitation mechanisms, such as fluorescence (radiative pumping), formation pumping, or shock excitation. These templates can easily be used with χ^2 minimization codes to assess the goodness-of-fit as functions of column density and doppler parameter. They provide a means for the user to concentrate on the fitting procedure without having to take on the computationally intensive task of calculating line profiles for a large number of absorbers. Such goodness-of-fit codes are under development and testing by many groups (c.f. Owens.f discussed in Lemoine et al. 2002 and Rachford et al. 2002), and some of these codes are available on-line³. The author will entertain inquiries into the use of beta versions that he is developing as time allows.

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A. Term Values and Thermal Population Distribution

Following Herzberg (1950), the ro-vibration energy levels (in wave-number units of cm^{-1}) of an an-harmonic oscillator is a sum of electronic, vibrational and rotational term values,

$$T(v, J) = T_e + G(v) + F(v, J) \quad (\text{A1})$$

where T_e is a constant for the given electronic state. $G(v)$ and $F(v, J)$ are given as expansions in $(v + \frac{1}{2})$ and $J(J + 1)$ respectively with $v = 0, 1 \cdots v_{max}$, $J = J_{min}, J_{min} + 1 \cdots J_{max}$,

$$G(v) = \omega_e(v + \frac{1}{2}) - \omega_e x_e(v + \frac{1}{2})^2 + \omega_e y_e(v + \frac{1}{2})^3 + \cdots, \quad (\text{A2})$$

$$F(v, J) = B_v J(J + 1) - D_v (J(J + 1))^2 + \cdots, \quad (\text{A3})$$

³<http://origins.colorado.edu/~tumlinso/h2/sw/sw.html>

and B_v and D_v are also given as expansions in $(v + \frac{1}{2})$,

$$B_v = B_e - \alpha_e(v + \frac{1}{2}) + \dots, \quad (\text{A4})$$

$$D_v = D_e + \beta_e(v + \frac{1}{2}) + \dots. \quad (\text{A5})$$

We reproduce in Table 1 the most significant term value constants for the $X^1\Sigma_g^+$, $B^1\Sigma_u^+$, and $C^1\Pi_u$ states collected by Huber & Herzberg (1979). They have also compiled a comprehensive list of the higher order constants of these expansions.

The $X^1\Sigma_g^+$ energy levels may be used in Boltzmann's law to determine the distribution of electrons among the ro-vibrational levels of the ground state under the assumption of thermal equilibrium. Following Draine & Bertoldi (1996) we write,

$$N(v, J)/g_J = N \exp\left[\frac{-hcT(v, J)}{kt}\right] \quad (\text{A6})$$

where N is a renormalization factor determined by first calculating the matrix elements $N(v, J)$ with $N = 1$ and then defining $N = \sum_{v=0}^{v_{\max}} \sum_{J=0}^{J_{\max}} N(v, J)$ for the renormalization. g_J is the degeneracy of the states where for even J (para- H_2) $g_J = 2J + 1$ and for odd J (ortho- H_2) $g_J = 3(2J + 1)$ under the assumption that the ortho to para ratio is 3.

B. Absorption Profiles

The formulae reproduced here are quite general and may be used in the calculation of any absorption line profile, atomic or molecular. The shape and strength of an absorption line depends on 5 independent constants, the oscillator strength $f_{v', v'', J', J''}$, the wavelength $\lambda_{v', v'', J', J''}$, the total lifetime of the upper state $\Gamma_{v', v'', J', J''}$, the doppler velocity $b = \sqrt{(2kT/m_{\text{H}_2})^2 + v_{\text{turb}}^2}$, and the column density of the lower state $N(v'', J'')$. The first 3 variables are set by quantum mechanics while the latter 2 are the quantities of interest along the line-of-sight. At first glance it would appear that we need to calculate separate templates for a grid of column densities and doppler parameters. However, this is not necessary because the cross-section profile is independent of column density so the optical depth scales linearly with column density. Consequently a series of optical depth templates, calculated with the same doppler velocity, can be directly scaled with column density, reducing our need for an optical depth series where the doppler parameter alone is varied.

Following Cartwright & Drapatz (1970), the normalized line profile as a function of wavelength (λ) for the absorbing transition of an electron in level $v'J' \leftarrow v''J''$ (which we will designate with an index i) maybe expressed as:

$$I_i(\lambda) = \exp(-\tau_i(\lambda)), \quad (\text{B1})$$

$$\tau_i(\lambda) = N(v'', J'') \sigma_i(\lambda), \quad (\text{B2})$$

$$\sigma_i(\lambda) = \sigma_i(\lambda_i) H(a, u), \quad (\text{B3})$$

$$\sigma_i(\lambda_i) \equiv \frac{\sqrt{\pi}e^2}{m_e c b} f_i \lambda_i, \quad (\text{B4})$$

$$H(a, u) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{a^2 + (u - y)^2}. \quad (\text{B5})$$

Here $H(a, u)$ is the Voigt function, a convolution of the a Maxwellian velocity distribution with a Lorentz profile (Rybicki & Lightman 1979). The dimensionless frequency is $u = \frac{v-v_i}{\Delta v_d}$ and $a = \frac{\Gamma_i}{4 \pi \Delta v_d}$ is the damping parameter. The continuous, discrete and doppler frequencies are $v = c/\lambda$, $v_i = c/\lambda_i$, and $v_d = (b/c)v_i$ (c is the speed of light, e is the electron charge in esu, m_e is the electron mass in grams, and b is defined above). The total lifetime of the upper state is a sum over all possible vibrational transitions out of the upper v' state and into the lower states $0 \leq v'' \leq 14$ such that $\Gamma_i = \sum_{v''=0}^{14} A_i$ where $A_i = \frac{2J'+1}{2J'+1} \frac{8 \pi^2 e^2}{m_e c \lambda_i} f_i$. The line core cross-section is $\sigma_i(\lambda_i)$ as the Voigt function has a value of $H(0, 0) = 1$ at line center (when $a \ll 1$ as is usually the case). $\sigma_i(\lambda)$ and $\tau_i(\lambda)$ are the cross-section and optical depth profiles, respectively.

In Figure 2 the curves-of-growth shown in red result from the numeric integration of $1 - \exp(-\tau_i(\lambda))$ over the complete wavelength interval of the profile, for a range of column densities, and discrete set of doppler parameters. The (well known) formulae for the linear, flat, and square root portion of the curves are overplotted (in black) to directly show the regions of validity for the approximations.

$$\frac{W_\lambda}{\lambda} = \frac{\pi e^2 N f \lambda}{m_e c^2} \quad (\text{B6})$$

$$= 2 \frac{b}{c} \left[\ln \left(\frac{\sqrt{\pi} e^2 N f \lambda}{m_e c b} \right) \right]^{\frac{1}{2}} \quad (\text{B7})$$

$$= \left[\frac{e^2 \gamma N f \lambda^2}{m_e c^3} \right]^{\frac{1}{2}} \quad (\text{B8})$$

These formulae are discussed in detail in (Spitzer 1978). It can be seen in Figure 2 that the formula for the flat portion of the curve-of-growth is low by approximately 6 – 8% with respect to the numeric calculation. An examination of (Münch 1968) shows this discrepancy can be accounted for by keeping the second order term in the asymptotic expansion of $\frac{W_\lambda}{\lambda}$ for large $\tau_0 = \left(\frac{\sqrt{\pi} e^2 N f \lambda}{m_e c b} \right) \gg 1$. The correction factor to $\frac{W_\lambda}{\lambda}$ is then $(1 + .2886/\ln \tau_0)$ and setting $\tau_0 \approx 50$ yields a 7% correction.

REFERENCES

- Aannestad, P. A., & Field, G. B. 1973, ApJ, 186, L29
 Abgrall, H., Roueff, E., Launay, F., Roncin, J. Y., & Subtil, J. L. 1993a, A&AS, 101, 273
 Abgrall, H., Roueff, E., Launay, F., Roncin, J. Y., & Subtil, J. L. 1993b, A&AS, 101, 323

- Andersson, B.-G., Wannier, P. G., & Crawford, I. A. 2002, MNRAS, 334, 327
- Cartwright, D. C., & Drapatz, S. 1970, A&A, 4, 443
- Draine, B. T., & Bertoldi, F. 1996, ApJ, 468, 269
- Federman, S. R. 1982, ApJ, 257, 125
- Herzberg, G. 1950, Spectra of Diatomic Molecules, New York: Van Nostrand Reinhold, 2nd ed.
- Huber, K. P., & Herzberg, G. 1979, Molecular Spectra and Molecular Structure IV: Constants of Diatomic Molecules New York: Van Nostrand-Reinhold, p. 249 – 250
- Lemoine, M. et al. 2002, ApJS, 140, 67
- McCandliss, S. R. 2001, ASP Conf. Ser. 247: Spectroscopic Challenges of Photoionized Plasmas, ed. by Gary Ferland and Daniel Wolf Savin, p. 523 – 527
- Meyer, D. M., Lauroesch, J. T., Sofia, U. J., Draine, B. T., & Bertoldi, F. 2001, ApJ, 553, L59
- Münch, G. 1968, Stars and Stellar Systems VII, Chicago: University of Chicago Press, p. 365
- Rachford, B. L. et al. 2002, ApJ, 577, 221
- Rybicki, G. B., & Lightman, A. P. 1979, New York: Wiley-Interscience, p. 291
- Sahnou, D. J. et al. 2000, ApJ, 538, L7
- Shull, J. M., & Beckwith, S. 1982, ARA&A, 20, 163
- Spitzer, L. 1978, Physical Processes in the Interstellar Medium, New York: Wiley-Interscience, p. 52
- Tumlinson, J. et al. 2002, ApJ, 566, 857

Fig. 1.— The transmission functions as derived for all the Lyman and Werner absorption lines originating from $J'' = 0,1,2,3,4$ longward of 900 \AA , top to bottom respectively. The vibrational transitions ($v' - 0$) are labeled above the lines with the Werner band label above the Lyman. The log columns are 21 and 20 for $J'' = 0,1$, 19 to 18 for $J'' = 2$, 17 for $J'' = 3$, and 16 for $J'' = 4$. These columns were chosen to be representative of the monotonically decreasing distributions commonly derived from far UV spectra.

Fig. 2.— Curve-of-growth diagram illustrating the regions of validity for each of the equivalent width approximation formulae. The numeric solution is in red, and the approximations are in black. Overplotted are the equivalent widths derived from direct numerical integration of the Lyman lines in the J=0 and J=1 templates for $b = 1, 2, 4, 8$, and 16 km s^{-1} showing the problem with the $b = 1 \text{ km s}^{-1}$ template. The

solid black horizontal line at the middle of the graph indicates roughly the boundary between resolved and unresolved (instrumentally broadened) line profiles, assuming the FUSE resolution is $R = 20000$. The dashed lines at the bottom of the graph indicate the 3σ equivalent width detection limits for continuum signal-to-noise ratios of 10 and 30 per resolution element. The placement of these lines was determined with the formula $W = 3(N/S)(\lambda/R)$.

Fig. 3.— On the right is a blowup of the Lyman R(0)(7-0) line as inserted into the common wavelength grid showing the truncation edge at -50 \AA from line center. The $\log N$ scalings of 21, 22 and 23 are overplotted. On the left is the same for Lyman R(0)(0-0), which has a smaller oscillator strength. The truncation edge is not as deep in the line on the right.

Fig. 4.— The variation of line profile for a fixed column of $\log N = 19$ in the R(0) (3-0), (2-0), (1-0) and (0-0) Lyman lines with two different doppler parameter (b) of 5 km s^{-1} and 10 km s^{-1} are overplotted. The shortward lines are very nearly the same, having become nearly fully damped they differ only in the core, while the (0-0) line for $b = 5 \text{ km s}^{-1}$ is still on the flat portion of the curve-of-growth. This illustrates how the higher vibrational transitions can be used to define the column and the lower vibrational transitions the doppler parameter b when the absorptions are making the transition from the flat portion of the curve-of-growth to the square root portion where the lines profiles become fully damped.

Fig. 5.— Curve-of-growth fitting example. The H_2 column densities and a doppler parameter have been derived from a curve-of-growth analysis. The fit for the (4-0) Lyman band fit is displayed in bottom right panel. An absorption line model containing lines from H I, D I, O I, and H_2 has been overplotted in each panel. The D I and O I models were also derived from curve-of-growth analysis while the H I model was “ χ -by-eye” from the Lyman- γ profile, which exhibits a damping wing.

Fig. 6.— χ^2 line profile fitting example. The rotational templates were used with an appropriate continuum to calculate χ^2 for selected portions of the line profiles of the (4-0) Lyman band. The upper panel shows how well the H_2 model from the (4-0) band fit reproduces the H_2 structures in the (5-0) band and constrains the location and degree of blending with lines of O VI, C II, O I and Ar I.

Table 1. Molecular Hydrogen Term Value Constants

State	T_e	ω_e	$\omega_e x_e$	B_e	α_e	D_e
$C^1\Pi_u$	100089.8	2443.77	69.524	31.362	1.664	2.23×10^{-2}
$B^1\Sigma_u^+$	91700.0	1358.09	20.888	20.015	1.1845	1.625×10^{-2}
$X^1\Sigma_g^+$	0	4401.21	121.33	60.853	3.062	4.71×10^{-2}

Table 2. Template File Arrays

Variable	Arrays		
λ_i	$\lambda_0 = 900$	\cdots	$\lambda_{58999} = 1489.99$
$\tau(\lambda_i)_{J''=0}$	$\tau(\lambda_0)$	\cdots	$\tau(\lambda_{58999})$
\vdots		\vdots	
$\tau(\lambda_i)_{J''=15}$	$\tau(\lambda_0)$	\cdots	$\tau(\lambda_{58999})$











