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ACCURATE HYDROGEN SPECTRAL SIMULATIONS WITH A COMPACT MODEL ATOM

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ABSTRACT

Many large-scale numerical simulations of astrophysical plasmas must also reproduce the hydrogen ionization and the resulting emission spectrum, in some cases quite accurately. We describe a compact model hydrogen atom that can be readily incorporated into such simulations. It reproduces the recombination efficiency and line spectrum predicted by much larger calculations for a very broad range of densities and temperatures. Uncertainties in hydrogen collision data are the largest source of differences between our compact atom and predictions of more extensive calculations and underscore the need for accurate atomic data.

Subject headings: atomic processes — plasmas

1. INTRODUCTION

Hydrogen is the most abundant element, and its physics dominates the conditions in a wide variety of galactic and extragalactic nebulae (Osterbrock 1989). Hydrogen's recombination efficiency and level populations must be computed with some precision, since its photoionization can be controlling the heating mechanism for many clouds, it is the dominant opacity for many forms of light, and H is often the dominant electron donor (Avrett & Loeser 1988; Rees, Netzer, & Ferland 1989; Netzer 1990). The line spectrum must be predicted with great precision if reliable abundance determinations are to be achieved (Martin 1988; Shields 1990; Pagel 1992). Modern spectral synthesis codes (see Kallman & Mushotzky 1985; Binette et al. 1993; Ferland et al. 1995; Netzer 1996) must incorporate complete simulations of the H atom if they are to be valid.

A number of physical processes affects hydrogen, including radiative and three-body recombination, photoionization and induced recombination, and collisional and radiative (spontaneous and induced) transitions between levels. Complete calculations of the physics of the hydrogen atom are intricate themselves (Brocklehurst 1971; Mathews, Blumenthal, & Grandi 1980; Drake & Ulrich 1980; Storey & Hummer 1995), and certainly cannot be incorporated into larger structure and spectral synthesis codes. These processes are important in the broad-line regions (BLRs) of quasars or any dense gas and so must be fully simulated.

Storey & Hummer (1995, hereafter SH), have completed full calculations of the hydrogen emission spectrum and recombination efficiency over a very broad range of temperature and density. Their calculations are for "case A" and "case B" conditions, with the 1000 lowest n levels and all l states included. These computations are likely to remain definitive for some time to come, and they made their results available electronically, along with a convenient interpolating program. Unfortunately, it is possible to incorporate model hydrogen atoms with only dozens, not hundreds or thousands, of levels into full spectral synthesis simulations. The problem is to define a compact model atom which retains the essential physics and agrees with the definitive calculations.

This paper outlines a model atom that can accurately reproduce the recombination efficiency and line emission with only a few dozen quantum levels and can be incorporated into large-scale structure simulations. The approach goes to the correct asymptotic limits and reproduces accurate results in intermediate conditions. We pay particular attention to obtaining accurate representations of emissivities of infrared lines. Surprisingly, the rates for collisions within the hydrogen atom appear to be the limiting factor on accuracy. Finally, we compare the idealized case B emissivity with results from a realistic BLR cloud model.

2. PHYSICAL PROCESSES AND THEIR SIMULATION WITH A COMPACT ATOM

Our model hydrogen atom consists of independent 1s, 2s, and 2p states and an arbitrary number of higher excited n-levels.

Both the low-density and LTE limits, as well as the intermediate "case A" and "case B" are well defined in the literature. Case B comes closest to simulating nature, and we concentrate on it here. For this approximation, all transitions involving the ground state are ignored, as is photoionization from excited states, collisional ionization and excitation from the ground and first excited states, fluorescent excitation, and all induced processes. These are normally included in our calculations but are disabled in the work presented below.

2.1. Photoionization, Radiative Recombination

Recombination to an infinite sum of bound levels must be included if the total recombination coefficient, and resulting ionization balance, are to be correct.

We have fitted radiative recombination coefficients for levels up to 15 using the Milne relation and photoionization cross sections taken from opacity project–related codes, as described in Ferland et al. (1992). The fit has the functional form

$$\alpha(n, T_e) = 10^{F(n, T_e)} T_e^{-1},$$

where

$$F(n, T_e) = \frac{a_n + c_n x + e_n x^2 + g_n x^3 + i_n x^4}{1 + b_n x + d_n x^2 + f_n x^3 + h_n x^4}$$

and

$$x = \log T_e.$$

Table 1 gives the coefficients used for the above equation, which are valid for the temperature range

$$2.8 \text{ K} \leq T_e \leq 10^{10} \text{ K}.$$
the first exponential integral & Stegun (Abramowitz 1965).

\[ \text{where } I \text{ is the ionization potential of the} \]

states at temperatures of 10,000 K. For levels 1

\[ n \]

The total recombination coefficient at these high tem-

\[ \text{peratures.} \]

Errors in individual recombination coefficient fits are

\[ \text{generally 1% with many less than 1% for lower excited} \]

\[ \text{levels. For quantum levels above 15 we use an asymptotic} \]

\[ \text{analytical formula from Allen (1973):} \]

\[ x_n = (3.26 \times 10^{-6}) n^{-3} T_e^{-3/2} \exp \left( \frac{\chi_n}{k T_e} \right) E_1 \left( \frac{\chi_n}{k T_e} \right), \]  

(2)

where \( \chi_1 \) is the ionization potential of the nth level and \( E_1 \) is
the first exponential integral (Abramowitz & Stegun 1965).

Errors in individual recombination coefficient fits are
generally 1%–2% with many less than 1% for lower excited
states at temperatures of 10,000 K. For levels 1 ≤ \( n \) ≤ 15
the largest errors are 5% at only the highest temperatures.
Equation (2), used for levels \( n \geq 16 \), breaks down at tem-
peratures greater than \( 10^8 \text{ K} \), however at these high tem-
peratures less than 2% of the total recombinations are to
levels greater than 16, so this does not introduce an error in
the total recombination coefficient at these high tem-
peratures.

The approach given above provides rates only for levels
explicitly included in our model atom and thus is an under-
estimate of the total recombination coefficient, a sum to
infinity. The total recombination coefficient must be accu-
rately computed to produce accurate ionization representa-
tions in the low-density limit. To compensate, the highest
five levels of the atom are assigned the remainder of the
recombination coefficient:

\[ x_n = x_B - \sum_{n=2}^{N-1} x_n, \]  

(3)

where \( x_B \) is the total case B rate (the sum of recombinations to
\( n = 2 \) and higher levels fitted with eq. [1] and coefficients
listed in Table 1), \( N \) is the total number of levels in the
compact model atom, and \( x_n \) is the recombination coeffi-
cient to the nth level. Although assigning the remaining
coefficient to the higher levels had the desired effect of
including all the possible recombinations, it also resulted in
the overpopulation of these levels. This caused a level inver-
sion and resulted in a strong maser and so was unphysical.
We topped off the atom with a band of levels rather than
the highest level to minimize this effect. The result of this
topping off of the atom is that the model atom reproduces
the \( x_B \) sum and the ionization balance at low densities to
very great precision.

2.2. Collisional Ionization, Three-Body Recombination

Collisional ionization and its reverse process, three-body
recombination, are important since they bring the atom
into LTE at high densities. Collisional ionization from the
ground state is taken from Arnaud & Rothenflug (1985).
For levels 2 and higher we use rate coefficients of Vriens
& Stueh (1980), who give a semiempirical fit between theory
and experiment for hydrogenic atoms. If the atom is in an
initial excited state \( |q\rangle \) with energy \( E_q = 13.6 \text{ eV/q}^2 \), then
the rate coefficient for ionization is

\[ K_q = \frac{9.56 \times 10^{-6} (kT_e)^{-1.5} \exp \left( -\frac{e_q}{kT_e} \right)}{e_q^{1.33} + 4.38e_q^{1.72} + 1.32e_q}, \]  

(4)

where \( e_q = E_q/kT_e \) is the Boltzmann factor with \( kT_e \) in eV,
and the equation is good for the values of \( kT_e \) given by
Vriens & Stueh (generally for temperatures greater than
\( 10^8 \text{ K} \)). For reference, the definitive SH calculations use
collision data from Burgess & Percival (1968). Chang,
Avrett, & Loeser (1991) discuss the uncertainties of the collis-
dion data for hydrogen. For intermediate levels this is easily
a factor of 2.

Figure 1 shows the total recombination coefficient for
three temperatures and a wide range of density. The solid
line presents the results with a 50-level atom, and the
dashed line presents the SH results. At low densities the
recombination coefficient is purely radiative, while three-
body recombination dominates the total at high density.
For low temperatures and intermediate densities the differ-
ences can be as great as 5%. Tests discussed below show
that the differences in our total recombination coefficient
and those of SH are due to the different collision data
assumed and so are a basic uncertainty.
Deﬁning a quantum state is given by the principle of detailed balance. Collisions between two levels, $|p\rangle$ and $|q\rangle$, with statistical weights $g_p$ and $g_q$, can be extended to any transition from any excited state. The recommended rate is $K_{pq}$ (Avrett, Loeser, & Chang, 1991), and can be extended to any transition from any excited state. The atom is in an initial upper level $|q\rangle$ and de-excites to a lower level $|p\rangle$ with energy $E_p = 13.6 \text{ eV}/p^2$ and energy difference $E_{pq} = 13.6 \text{ eV}/(1/p^2 - 1/q^2)$; then the de-excitation rate coefficient is given by

$$K_{pq} = \frac{1.6 \times 10^{-7} (kT_e)^0.5 g_p g_q}{kT_e + \Gamma_{pq}} \times \left[ A_{pq} \ln \left( \frac{0.3kT_e}{\mathcal{R}} + \Delta_{pq} \right) + B_{pq} \right],$$

where $g_p = 2p^2$ and $g_q = 2q^2$ are the statistical weights. Defining $s = |p - q|$, we have

$$\Delta_{pq} = \exp \left( \frac{-B_{pq}}{A_{pq}} \right) + \frac{0.06s^2}{pq^2},$$

and

$$\Gamma_{pq} = \frac{\mathcal{R} \ln(1 + q^3 kT_e/\mathcal{R})[3 + 11(s/q)^2]}{(6 + 1.6ps + 0.3/s^2 + (0.8p^{1.5}/s^{0.5})|s - 0.6|)},$$

$$A_{pq} = \left( \frac{2\mathcal{R}}{E_{pq}} \right) f_{pq},$$

and

$$B_{pq} = \frac{4\mathcal{R}^2}{p^3} \left( \frac{1}{E_{pq}^2} + \frac{4E_{pq}}{3E_q^3} + \frac{b_p}{E_q^2} \right),$$

with

$$b_p = \frac{1.4 \ln p - 0.7}{p} - \frac{0.51}{p^2} + \frac{1.16}{p^3} - \frac{0.55}{p^4}.$$

The value $\mathcal{R}$ is the Rydberg constant and $kT_e$ is in eV. $f_{pq}$ is the absorption oscillator strength given by Johnson (1972). For comparison SH use data from Percival & Richards (1978). Again, differences can easily be a factor of 2 and are a basic problem (Chang, Avrett, & Loeser, 1991).

Case B does not deﬁne the populations of the $n = 1$ or $n = 2$ levels, so collisions from these levels are not included in the comparisons made below.

### 2.4. Radiative Cascade

This is the most diﬃcult process to simulate, and the only one whose treatment is nonstandard, because the branching ratios from each level depend on both density and temperature. Physically, captures tend to occur to higher angular momentum, $l$, levels. As electrons cascade downward they further tend to “bunch up” at the highest possible $l$-values because of the $\Delta l = 1$ selection rule. Distant collisions with slow-moving protons tend to distribute the electron density population according to statistical weight. As a result, the actual distribution of populations among the $l$-levels will have a density dependence, and the branching ratios from a particular level will too.

The dashed line in Figure 2 shows the $P_a$ to $H\beta$ ratio from SH for three temperatures. The lines have a common upper level, and so the intensity ratio is proportional to the $4-3/4-2$ branching ratio. The lines are observationally important since both are strong and can be readily detected, and the ratio has a large dependency on the density and temperature of the gas. There are two simple limits; the well $l$-mixed, high-density limit with $P_a/H\beta = 0.277$ (at all temperatures) corresponding to the Seaton (1959) recombination spectrum, and the low-density limit with $P_a/H\beta = 0.339$ (at 10,000 K), where $l$-mixing collisions are negligible (corresponding to the calculations presented by Pengelly 1964 and Martin 1988).

We deﬁned a transition probability from each excited level in terms of a constant total case B lifetime (the sum of the Einstein $A$’s for the upper level minus the ground-state transition) and a set of branching ratios which depend on density and temperature, as the solid line in Figure 2 shows. These branching ratios were obtained by ﬁtting the SH...
TABLE 2

<table>
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<th>q</th>
<th>p</th>
<th>n_{min}</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
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<td>7</td>
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<td>0.0033</td>
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<td>0.4378</td>
<td>-0.0145</td>
</tr>
<tr>
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<td>4</td>
<td>7</td>
<td>0.0752</td>
<td>0.0244</td>
<td>0.1636</td>
<td>0.1619</td>
<td>0.0000</td>
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<td>0.1750</td>
<td>0.2684</td>
<td>-0.0090</td>
</tr>
<tr>
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<td>5</td>
<td>0.2315</td>
<td>-0.0180</td>
<td>0.2190</td>
<td>0.3407</td>
<td>-0.1284</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>6</td>
<td>0.8889</td>
<td>-0.0615</td>
<td>0.2450</td>
<td>0.4915</td>
<td>-0.2232</td>
</tr>
</tbody>
</table>

RESULTS

The atom has been incorporated into the radiative equilibrium code CLOUDY (Ferland 1996). We have left the total number of levels of the hydrogen atom as an option. More levels generally produce a better agreement with the SH results, but at the expense of longer execution times. Tests show that lower temperatures require more levels, because the highest level must be well within $kT_e$ of the continuum for three-body recombination to achieve its full efficiency. A flexible choice in the number of levels was a major reason for the chosen structure of the model atom. For all of the results shown here a 50-level atom was used.

Figure 3a shows a contour plot of the emissivity of Hβ (in units of $4\pi j_{\beta}/n_e n_c$) for temperatures greater than $10^4$ K and the full range of densities considered by SH. The Hβ emissivity varies by 5 orders of magnitude for this range in conditions. Figure 3b shows a ratio of this work and that of SH. For nebular temperatures (5000–20,000 K) and all densities, the differences are less than 2%. For low temperatures ($<3000$ K) and low densities ($<10^17$ cm$^{-3}$), the general agreement is to within 6%. In this limit the differences are due to our use of well $l$-mixed Einstein A’s for the higher levels (see § 2.4). At low temperatures, captures are mainly to these levels, which are not actually mixed at low densities. This is a basic limitation of our approach.

Uncertainties in the collision data (see § 2.2) are the main reason our atom does not agree exactly with SH at low temperatures ($<3000$ K) and high densities ($>10^{18}$ cm$^{-3}$). We quantify the basic uncertainties by modifying the collisional rate coefficients from Vriens & Smeets by a factor of 2, the representative uncertainty discussed by Chang, Avrett, & Loeser (1991). Figure 3c shows the ratio of our predictions with and without this scale factor and so shows effects of these uncertainties. Results changed by nearly a factor of 2 at low temperatures and high densities, in response. We attribute the differences in our results and SH at low temperature and high densities to the fact that we use different sources for the collision data. The results for nebular conditions (5000–20,000 K) are affected very little, and we agree with SH very well.

Figure 4 shows our results with SH for four Balmer lines at $T_e = 10^4$ K relative to Hβ. At log $n_e = 2.0$ we calculate the Balmer decrement, $H_\alpha/H_\beta/H_\gamma/H_\delta$, to be 2.866/1.0/0.473/0.262, and at log $n_e = 14.0$, it is 3.548/1.0/0.388/0.189. The SH results for the same densities are 2.86/1.0/0.468/0.259 and 3.41/1.0/0.387/0.188, respectively.

Figure 5 shows the intensities of two observationally important infrared emission lines at $T_e = 10^4$ K relative to Hβ. They agree with SH to typically within 1%–2%, with
TABLE 3
FITS OF THE BRANCHING RATIOS FOR UPPER LEVELS GREATER THAN 7

<table>
<thead>
<tr>
<th>Lower-Level $p$</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
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<td></td>
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</tr>
<tr>
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<td>0.0523</td>
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<td>0.7604</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$B$...</td>
<td>0.0465</td>
<td>0.0227</td>
<td>0.0080</td>
<td>-0.0049</td>
<td>-0.0206</td>
<td>-0.0518</td>
<td></td>
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</tr>
<tr>
<td>$C$...</td>
<td>0.2096</td>
<td>0.1565</td>
<td>0.1352</td>
<td>0.1322</td>
<td>0.1490</td>
<td>0.2175</td>
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</tr>
<tr>
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</tr>
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<tr>
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<td>0.0000</td>
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<td>0.0655</td>
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<td>0.1380</td>
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*a* $q$ is the upper level.
the largest errors being 5%. Tests show that this accuracy is
typical for lines produced by levels lower than 15, the
highest level we attempted to take account of variable $l$
mixing.

The case B approximation does not include the effects of
the ground and the first excited states by design, so these
results cannot be directly applied to dense clouds. Among
the processes which were disabled for the comparisons
above were continuum pumping, photoionization and
induced recombination from excited states, and collisional
excitation from the ground or first excited states. For dense
clouds such as the BLR of a quasar, these are very impor-
tant processes.

Table 4 compares case B with this work for $10^4$ K and an
electron density of $10^{11}$ cm$^{-3}$, typical BLR conditions from
Ferland et al. (1992). Column (1) lists the line labels, column
(2) contains the case B ratios with respect to H$\beta$, and
column (3) contains results from our compact atom with all
induced processes disabled. Columns (4) and (5) show the
effects of multiplying the collision data for levels higher
than two by factors of 2 and 0.5, respectively. Clearly the
results are sensitive to these uncertain numbers. Column (6)
shows the results of enabling induced photoionization and
recombination and stimulated emission for a continuum
shape and an ionization parameter (ratio of photon density
to hydrogen density) of 0.1, given by the standard BLR

**Fig. 3**—Contour plots. (a) The log of the total H$\beta$ emissivity (in units of $4\sigma j / n_e n_p$) for all densities and temperatures. Solid lines are 1 dex increments and
dashed lines are 0.2 dex steps. (b) Ratio of our predicted H$\beta$ emissivity to SH; 10% increments are solid lines, and 2% steps are dashed lines. (c) Same as (b),
but with the collisional atomic data multiplied by 2, as described in the text. In (c) the solid lines are 20% differences and the dashed lines 10%. Factor of 2
changes result for some parameters.
model from Ferland et al. (1992). Column (7) has collisions from the ground and first excited states included in the calculation. Column (8) lists the results of allowing the Lyman lines to be optically thin.

Finally, the results of a complete calculation are shown in column (9). This solves for the energy balance and so has a depth-dependent temperature (the mean is close to $10^4$ K). It again assumes a hydrogen density of $10^{11}$ cm$^{-3}$, has a

![Fig. 4.—Selected ratios of Balmer lines relative to H$\beta$ for $10^4$ K and the full range of density. This work is shown as solid lines and the SH results as dashed lines.](image)

![Fig. 5a.—Two examples of important infrared lines shown at $10^4$ K and the full range of density. **Solid lines:** this work, **dashed lines:** SH. (a) Br$_\gamma$ to H$\beta$; (b) H$\alpha$/H$\beta$. H$\alpha$ is Humphries $\alpha$, the transition from level 7 to level 6 in hydrogen.](image)

![Fig. 5b](image)
TABLE 4

<table>
<thead>
<tr>
<th>LINE</th>
<th>CASE B</th>
<th>1(^a)</th>
<th>2(^b)</th>
<th>3(^b)</th>
<th>4(^c)</th>
<th>5(^c)</th>
<th>6(^d)</th>
<th>BLR(^h)</th>
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<tr>
<td>H(\beta)</td>
<td>1.84((-25))</td>
<td>1.80((-25))</td>
<td>1.95((-25))</td>
<td>1.64((-25))</td>
<td>2.94((-25))</td>
<td>3.03((-25))</td>
<td>1.25((-25))</td>
<td>1.04((-27))</td>
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<tr>
<td>Ly(\alpha)</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
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<tr>
<td>H(\alpha)</td>
<td>2.55</td>
<td>2.56</td>
<td>2.51</td>
<td>2.61</td>
<td>6.71</td>
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<td>H(\delta)</td>
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<td>0.570</td>
<td>0.594</td>
<td>0.545</td>
<td>0.4511</td>
<td>0.443</td>
<td>0.630</td>
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<tr>
<td>H(\iota)</td>
<td>0.394</td>
<td>0.395</td>
<td>0.406</td>
<td>0.363</td>
<td>0.268</td>
<td>0.262</td>
<td>0.480</td>
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<tr>
<td>Pa(\alpha)</td>
<td>0.277</td>
<td>0.277</td>
<td>0.277</td>
<td>0.277</td>
<td>0.277</td>
<td>0.277</td>
<td>0.277</td>
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<td>Pa(\beta)</td>
<td>0.168</td>
<td>0.169</td>
<td>0.175</td>
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<td>Br(\alpha)</td>
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<td>0.0651</td>
<td>0.0679</td>
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<td>0.0515</td>
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<td>H(\alpha)</td>
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<td>0.0093</td>
<td>0.0091</td>
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<td>0.0058</td>
<td>0.0056</td>
<td>0.0122</td>
<td>0.0022</td>
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\(^a\) Case B results are from SH.
\(^b\) CLOUDY with physical processes disabled as described in text.
\(^c\) Same as col. (3), but with collision data times 2.
\(^d\) Same as col. (3), but with collision data times 0.5.
\(^e\) Induced processes enabled.
\(^f\) Collisions between 2\(s\) and 2\(p\) electrons included.
\(^g\) Case B assumption turned off.
\(^h\) Simple BLR cloud as described in the text.

H\(\beta\) emissivity in units of ergs cm\(^{-3}\) sec\(^{-1}\); number in parentheses is the exponent.

In summary, we find that a compact hydrogen atom can reproduce quite well the hydrogen emission spectrum calculated with a more extensive model atom at most temperatures and densities. Our results underscore the points made by Chang, Avrett, and Loeser (1991), indicating the need for more accurate collisional rate coefficients.

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