TRANSITION PROBABILITIES FOR THE UV0.01 MULTIPLET IN N III

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ABSTRACT

We report on large-scale ab initio multiconfiguration Hartree-Fock calculations for the UV0.01 multiplet, 2s2p2 2P0–2s2p4 4P1, in N iii. The resulting transition probabilities agree very well with recent semiempirical calculations, and the lifetimes for two of the three upper levels agree with experiments. The deviation for the third level is discussed.

Comparisons made with the highest quality IUE echelle spectra available—those of RR Tel and V1016 Cyg (both photoionized sources with electron densities below 10^6 cm^-3)—show that computed branching ratios of lines sharing a common upper level are in agreement with observations to within uncertainties of ±10%.

High-quality solar limb data or stellar data from the Hubble Space Telescope could, in principle, be used to determine whether the theoretical or measured lifetimes for the discrepant level are in error. Unfortunately, stellar data for high-density plasmas (N_e > 10^{11} cm^-3 are needed) do not yet exist, and existing solar data lack the photometric precision to address this problem.

Subject headings: atomic data — stars: individual (RR Telescopii, V1016 Cygni) — ultraviolet: general — ultraviolet: stars

1. INTRODUCTION

The intercombination lines of boron-like ions are often used for electron density determination of different low-density astrophysical plasmas (Judge et al. 1993). Examples of these are the solar and stellar chromosphere and transition regions (Feldman & Doschek 1979; Stencel et al. 1981), symbiotic stars (Nussbaumer & Storey 1979), and planetary nebulae (Keenan et al. 1994). The determined electron densities are very sensitive both to the relative transition probabilities and to the collision rates, since the predicted relative intensity only changes by a factor of 2 over a range of two orders of magnitude of electron density (Feldman & Doschek 1979). Given that the collision rate calculations are based on the same, but necessarily more restricted, set of wavefunctions as used for the radiative rates, it is clear that the first step in assessing the accuracy of the computed line ratios as density diagnostics must involve determining the reliability of the atomic wavefunctions and radiative rate coefficients. The need for accurate radiative data is therefore great.

These lines are also of great interest for basic atomic structure theory since their transition rates depend strongly on a correct treatment of a number of different properties of the ions. These electric dipole transitions are forbidden in a basic LS-coupling model and become allowed only through spin-induced interactions. Hence the model used needs to treat both the different transition and fine-structure properties accurately.

We have initiated a project to compute these rates, using highly systematic multiconfiguration Hartree-Fock (MCHF) techniques (Froese Fischer 1991). By including relativistic effects through the Breit-Pauli approach, we believe that we can compute oscillator strengths of intersystem lines to a very high accuracy. This method has been used successfully to obtain a number of different atomic parameters recently (Brage & Froese Fischer 1993; Jönsson 1993). In an earlier publication, results were reported on the C ii intersystem and allowed lines (Froese Fischer 1994). In this paper we will extend the work to investigate N iii and make comparisons with laboratory measurements and astrophysical spectra.

2. METHOD OF CALCULATION

The main advantage of using an ab initio, systematic method is that it allows for independent checks of accuracy and convergence. Through this it is possible to estimate the accuracy of the calculations and to conclude whether all important contributions have been included. The model is based on an expansion of the atomic state function (ASF) in a linear combination of configuration state functions (CSFs),

\[ \Psi(\gamma LS) = \sum_i c_i \Phi(\alpha_i LS) , \]

(1)

in the nonrelativistic LS model, where \( \alpha \) specifies a configuration, the coupling, and any other quantum numbers needed to uniquely specify the CSF. If spin-dependent, relativistic effects are included we get

\[ \Psi(\gamma LSJ) = \sum_i c_i \Phi(\alpha_i LSJ) . \]

(2)

The CSFs are constructed, according to antisymmetry and angular momentum rules, as linear combinations of products of one-electron spin orbitals:

\[ \phi(nl m_l m_s; r) = P(nl; r)Y(lm_l; \theta \phi)\gamma(m_s) . \]

(3)

The unknowns are the radial functions, \( P(nl; r) \), and the configuration interaction (CI) coefficients, \( c_i \). The former are determined by solving a set of coupled integraldifferential equations, according to the MCHF scheme. This is done in the nonrela-
tivistic LS framework on a given term. The c coefficients are obtained from diagonalizing the Breit-Pauli Hamiltonian energy matrix in a final J-dependent CI calculation.

In both these parts of our calculations we are faced with an important task, to choose the set of CSFs to include in the CI expansions. A number of different approaches have been designed to systematize this choice. In the earlier days of atomic structure computing it was essential to keep the size of the expansion to a minimum, and CSFs were included more or less one by one according to what previous experience from similar cases indicated would be important. In more recent years, we have attempted to develop a methodology based on the idea of an active space of CSFs. The advantage of this is that it guarantees that all important contributions will be included and opens up the possibility for highly systematic calculations and thereby the estimation of the uncertainties of the results. For a more detailed account of these methods, we refer the reader to a recent review (Brage & Froese Fischer 1993).

The systematics will be defined in two different ways. First, we will attempt to use a number of increasingly sophisticated models, including more and more correlation, to investigate the convergence of models. Second, within each model we increase stepwise the active set of orbitals, in a systematic way, to ensure convergence of the results.

The models are defined by the constraints on the CSFs. The important step is to recognize different parts of the electron cloud in the ions and to define the corresponding subshells to be of valence or core type. The former usually consists of a few open, outer shells, while the latter is defined by inner shells that, to quite good approximation, can be treated as close and spherically symmetric. In the case of boron-like ions, where the two lowest configurations are of the forms

\[ 1s^22s^22p \quad \text{and} \quad 1s^22s2p^2, \]

it is natural to define the three outermost electrons as belonging to the valence subshells, while the 1s2 constitutes the core. The most important contributions to transition-type atomic properties arise from correlation between the valence electrons. This is represented by CSFs of the form

\[ 1s^2n_1l_1n_2l_2n_3l_3. \]

The second most important contribution comes from core polarization, taken into account by including CSFs of the form

\[ 1snl_1l_2n_2l_3n_3l_4. \]

The final model would involve adding the core-core correlation, by also including CSFs that are completely unrestricted in the choice of orbitals, and is formed as all possible combinations of five orbitals from the active set. This type of calculation will grow in size very quickly, and it is therefore desirable to monitor different quality criteria to see if this last step can be avoided.

There are a number of different types of quality criteria for a model that we will use. One possibility is to investigate other, known, properties that influence the accuracy of the property we wish to determine. Since our goal here is to compute transition probabilities for, primarily, \( 2s2p^2 P_J - 2s2p^2 P_J \), intercombination lines, we will monitor three other properties. First, the excitation energy of the \( 4P \) directly influences the transition probability, since the latter is proportional to \( 1/l^3 \). The second property to monitor is the splitting between interacting terms. The intercombination lines are induced primarily through two different effects: (1) spin-induced mixing of the \( 4P \) with the \( 3S, 2P, \) and \( 2D \) in the same configuration \( 2s2p^2 \) and (2) spin-dependent mixing between the \( 2s2p^2 P \) and the \( 2p^3 4S \), induced by the strong CI mixing of \( 2s^2 2p^2 \) and \( 2p^3 2P \). The energy differences between these interacting terms have to be accurately represented by our model. The third property to monitor is the fine structure of the different terms. This serves as quality control of the spin-dependent interaction between the terms since it is given by the same type of integrals.

The fact that the radial functions are determined in a nonrelativistic LS calculation, while in the final model a number of LS terms have to be included, makes a proper choice of optimization technique important. The radial functions might depend strongly on which term they have been optimized on, that is, which term has been used to define the MCHF equations. For example, the 2p orbital of the \( 2p^3 4S \) is quite different from the 2p of the ground term \( 2s^2 2p^2 P \). This term dependency has to be included in our calculations in some way. To retain the systematic nature of the calculation, we have chosen a method in which all orbitals with \( n \leq N \), labeled the "inner" set, are included for one term, and a set with \( n = N + 1 \), the "outer" set, optimized on a second. For the odd states, the first term is \( 2s^2 2p^2 P \) and the second \( 2p^3 4S \), while for the even states we use \( 2s2p^4 P \) and \( 2S \). The same set as for \( 2s2p^2 \) is used for \( 2p^3 4P \) and \( 2D \). In the tables the different steps are labeled by the maximum main quantum numbers for the two sets, \( (N, N + 1) \). As an example, in the step labeled \( (3, 4) \) we optimize the \( 2s, 2p, 3s, 3p, \) and \( 3d \) on the \( 2s2p^2 P \) for the odds and on \( 2s2p^2 4P \) for the evens. These inner orbitals are kept fixed, and an extra set consisting of \( 4s, 4p, \) and \( 4d \) is added and optimized on the \( 2p^3 4S \) and \( 2s2p^2 2S \), respectively. Note that only the same \( l \) quantum numbers as in the inner set are used, and \( 4f \) is therefore not included. For the \( 2s2p^2 2D \) and \( 2P \) we assume that this orbital set is sufficient.

This stepwise procedure is performed for two different models. The first one only considers outer correlation, and we include CSFs of the form

\[ \{1\}^2 \{2, 3, \ldots, n_{\text{max}}\}^3, \]

which implies that all CSFs have a closed 1s2 shell and that the outer three are any distribution of orbitals with \( n \in \{2, 3, \ldots, n_{\text{max}}\}. \) The second model also includes core polarization. For this we include all CSFs of the form

\[ \{1\} \{1, 2, 3\}^2 \{2, 3, \ldots, n_{\text{max}}\}^2. \]

We are forced to use this somewhat more restricted form, where at least three orbitals have \( n \) quantum numbers between 1 and 3, due to orthogonality constraints for transition calculations. These orbitals are common for all different terms, as obtained in an MCHF calculation for the \( 2s2p^2 4P \). The resulting excitation energies from some of our calculations are given in Table 1. We only show the final \((5, 6)\) step for outer correlation, but to illustrate the convergence of the calculations we give all four steps for the core polarization models.

3. RESULTS

As we already have discussed, it is possible to use other properties to determine the quality of our calculations. In addition to this we will investigate theoretical uncertainty indicators, in the form of agreement between the results from models
using different forms (or gauges) for the transition operator. A third test will be the convergence of the results from a set of models, and from a set of approaches within the model.

The most obvious “other properties” that influence the accuracy of the intersystem lines are the different energy properties that can be deduced from Table 1. Although it is all too simplistic an expression for actual computations, the first-order formula for spin-induced transitions is useful to estimate uncertainties in the computed transition probabilities:

\[ A_{	ext{sf}} = \left( \frac{\lambda_{\text{sd}}}{\lambda_{\text{sd}}} \right)^3 c_1^2 A_a, \]  

where the subscripts “sf” and “a” on the rates and wavelengths denote spin-forbidden and allowed transitions, respectively. The \( c_1 \) is the CI coefficient of the corresponding doublet state, in the quartet. This is given by, to first order,

\[ c_1^2 \propto \left( \frac{E_{\text{PS}}}{E_{\text{quartet}} - E_{\text{doublet}}} \right)^2, \]

that is, the square of the ratio of the fine-structure and term-splitting energies.

If we start with the energy differences between interacting terms, it is clear from Table 1 that the inclusion of core polarization is important, especially for the \( 2s^2p^2 P_{1/2} - 2p^3 P_{3/2} \) splitting. The deviation from experimental values is less than 0.5% for all cases in the final calculation. The contribution to the uncertainty of the intersystem transition probabilities is therefore less than 1% from this source.

The wavelength is also uncertain to less than a few tenths of a percent, and the uncertainty contributions are therefore the same order of magnitude as from the term splittings.

The fine structure of different terms is very accurately represented by our approach. Again, it is essential to include core polarization to bring the agreement with experiment to within a percent. The only exception is the \( 2s^2p^2 P_{1/2} \), but we believe that this is not a fine-structure effect, but rather a secondary effect from configuration interaction. The contribution to the fine structure from the spin-orbit term, which is the dominating one, is zero in the first-order approach, and the prediction of the \( (J = 5/2) - (J = 3/2) \) splitting depends on other factors.

The final property to investigate is the transition rates, \( A_{\text{sf}} \), for allowed transitions. These have been determined experimentally in some cases (Dumont, Biemont, & Grevesse 1974). These investigations were performed using the beam-foil technique without a careful treatment of cascades. It was later shown that the uncertainty can therefore be quite large and that the lifetime is often overestimated due to long-lived cascades (Curtis, Berry, & Bromander 1971; Engström 1982). The uncertainties in these experimental values are certainly much larger than in the theoretical calculations reported here.

An independent test of accuracy is the agreement of our results using two different forms of the transition operator, the length and velocity forms. In Table 2 we show the results from final calculations without and with core polarization. In all cases the difference is 1% or less, which induces the same uncertainty in the spin-forbidden transition rate.

We give the resulting transition probabilities for the intersystem lines in Table 3, from the different steps in our approach and other calculations and experiments. A reasonable estimate.

### Table 1

<table>
<thead>
<tr>
<th>Level</th>
<th>A Initi MCHF</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Outer*</td>
</tr>
<tr>
<td></td>
<td>(5, 6)*</td>
</tr>
<tr>
<td>( 2s^2p^2 )</td>
<td>0.00</td>
</tr>
<tr>
<td>( 4P_{3/2} )</td>
<td>170.0</td>
</tr>
<tr>
<td>( 2P_{3/2} )</td>
<td>57302.4</td>
</tr>
<tr>
<td>( 4P_{1/2} )</td>
<td>57360.4</td>
</tr>
<tr>
<td>( 4P_{1/2} )</td>
<td>57439.3</td>
</tr>
<tr>
<td>( FS(2P^p) )</td>
<td>136.9</td>
</tr>
<tr>
<td>( 4P_{3/2} )</td>
<td>101578.2</td>
</tr>
<tr>
<td>( FS(4P^p) )</td>
<td>6.1</td>
</tr>
<tr>
<td>( 2S_{1/2} )</td>
<td>131575.3</td>
</tr>
<tr>
<td>( 2P_{3/2} )</td>
<td>143703.5</td>
</tr>
<tr>
<td>( 3P_{3/2} )</td>
<td>147412.9</td>
</tr>
<tr>
<td>( FS(4P^p) )</td>
<td>107.5</td>
</tr>
</tbody>
</table>

\* From Eriksson 1958; Edlén et al. 1969.
\* Outer correlation only.
\* Including core polarization.
\* \((N, N + 1)\) implies that orbitals with \( n \leq N \) are included for the “inner” terms \((2s^2p^2 P \text{ and } 2s^2p^2 \text{ } 4P)\) and \( n \leq N + 1 \) for the rest. See text.

*Fine structure splitting.*

### Table 2

<table>
<thead>
<tr>
<th>Transition</th>
<th>Present Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 2s^2p^2 P - 2s^2p^2 D )</td>
<td>0.7481/0.8107</td>
</tr>
<tr>
<td>( 2s^2p^2 P - 2s^2p^2 S )</td>
<td>0.4932/0.5229</td>
</tr>
<tr>
<td>( 2s^2p^2 P - 2s^2p^2 P )</td>
<td>2.4391/2.6294</td>
</tr>
<tr>
<td>( 2s^2p^2 P - 2p^3 P )</td>
<td>1.7693/1.9247</td>
</tr>
</tbody>
</table>

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of the convergence is to within a few percent. The total errors in the final values, therefore estimated to be less than 5%. The semiempirical configuration interaction (CIV3) calculation by Bell et al. (1994) was performed parallel to the present one. The core polarization was not included in that work, which led to a number of inaccuracies in the ab initio results. The energy splitting was corrected for by adding small corrections to the diagonal elements. Since the core polarization also affects the fine structure, significantly, the CIV3 results were $\sim 3\% - 4\%$ too small. If we adjust the resulting intersystem transition probabilities correspondingly, according to equation (4), we arrive at the results in the “Adjusted” under CIV3 in Table 3. These are in excellent agreement with the MCHF values. It seems that the main effects of the core polarization are on fine structure and excitation energies.

The earlier CIV3 calculation by Stafford, Hibbert, & Bell (1993) used only a semiempirical, one-body spin-orbit operator for all $J$-dependent effects. This is insufficient, as is pointed out by Bell et al. (1994) since two-body effects (spin-orbit and spin-other-orbit) are quite important for light elements such as nitrogen.

A comparison with experimental lifetimes, obtained by Fang, Kwong, & Parkinson (1993), shows a more puzzling discrepancy. For the longest lived state, $^4P_{1/2}$, the agreement is excellent, and it is fair for the medium-life $^4P_{5/2}$. The shortest lived $^4P_{1/2}$ level shows a larger discrepancy, of $30\% - 40\%$. It is plausible that it is the most difficult to measure, due to its shorter lived character, but similar methods seem to successfully deal with even shorter lived states in, for example, P II (Calamai, Han, & Parkinson 1992).

On the theoretical side, the accuracy points at the interaction between the $^4P_{1/2}$ and the $^3S_{1/2}$. The radial integrals for the resonance line from the latter are affected by a strong cancellation effect, between the contributions from the $2s^2p^2\,P - 2s^2p\,P$ and $2s^2p^2\,P - 2s^3\,S$ components. If the “dynamics” of this cancellation, and its effects on the intercombination lines, is responsible for a large error in the theoretical transition rates, it seems odd that two quite different methods agree so well (the adjusted CIV3 and the MCHF). Another fact that supports the accuracy of the calculations is the success for C II (Froese Fischer 1994), where results from MCHF calculations are close to the lower limits of the error estimates on the experimental value.

We give in Table 4 the oscillator strengths for a number of fine-structure transitions in N III.

### Table 3

<table>
<thead>
<tr>
<th>Transition</th>
<th>$\lambda$ (Å)</th>
<th>Outer (5, 6)</th>
<th>Core Polarization (3, 4)</th>
<th>(4, 5)</th>
<th>(5, 6)</th>
<th>(6, 7)</th>
<th>Experiment by FANG</th>
<th>CIV3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^2P_{3/2} - ^4P_{5/2}$</td>
<td>1749.674</td>
<td>265.1</td>
<td>226.2</td>
<td>265.6</td>
<td>283.1</td>
<td>281.8</td>
<td>308 ± 22</td>
<td>260.0</td>
</tr>
<tr>
<td>$^2P_{3/2} - ^4P_{3/2}$</td>
<td>1752.160</td>
<td>58.7</td>
<td>53.4</td>
<td>61.0</td>
<td>64.3</td>
<td>65.1</td>
<td>...</td>
<td>60.2</td>
</tr>
<tr>
<td>$^2P_{1/2} - ^4P_{1/2}$</td>
<td>1748.822</td>
<td>9.1</td>
<td>7.0</td>
<td>8.6</td>
<td>9.3</td>
<td>9.1</td>
<td>...</td>
<td>8.8</td>
</tr>
<tr>
<td>Total ($^2P_{3/2}$)</td>
<td>...</td>
<td>67.8</td>
<td>60.4</td>
<td>69.6</td>
<td>73.6</td>
<td>74.2</td>
<td>74.5 ± 5.4</td>
<td>69.0</td>
</tr>
<tr>
<td>$^2P_{3/2} - ^4P_{5/2}$</td>
<td>1753.986</td>
<td>356.7</td>
<td>328.7</td>
<td>351.2</td>
<td>368.8</td>
<td>371.7</td>
<td>...</td>
<td>361.5</td>
</tr>
<tr>
<td>$^2P_{1/2} - ^4P_{1/2}$</td>
<td>1748.646</td>
<td>339.8</td>
<td>314.7</td>
<td>340.4</td>
<td>356.9</td>
<td>360.9</td>
<td>...</td>
<td>346.8</td>
</tr>
<tr>
<td>Total ($^2P_{3/2}$)</td>
<td>...</td>
<td>696.5</td>
<td>643.4</td>
<td>691.6</td>
<td>725.7</td>
<td>732.6</td>
<td>1019 ± 64</td>
<td>708.3</td>
</tr>
</tbody>
</table>

* Edlén et al. 1969.
* Present, see text and Table 1.
* Superstructure calculations (Nussbaumer & Storey 1979; Eissner, Jones, & Nussbaumer 1974).
* Fang et al. 1993.
* Bell et al. 1994.
* Results from Bell et al. 1994, adjusted for experimental fine structure.

4. LINE RATIOS FROM SPECTRA OF ASTRONOMICAL PLASMAS

Given the large discrepancy between the $^4P_{1/2}$ lifetime measured by Fang et al. (1993) and the present calculations, one can turn to astronomical sources for further information. First we examined solar spectra, and then we turned to data from the International Ultraviolet Explorer (IUE) archive. To our knowledge, no suitable data for the N III multiplet have yet been obtained with the Goddard High Resolution Spectrometer (GIRS) on Hubble Space Telescope.

Attempts to determine atomic parameters from astronomical sources are fraught with potential problems, but there are specific conditions under which very accurate constraints on the parameters can be determined. First, the data must be well calibrated and relatively noise-free. Second, one must be able to determine the influence of blended lines (emission and absorption). Third, one must be able to demonstrate that the emergent line intensities, or ratios thereof, are insensitive to unknown or poorly determined plasma properties.

For the case of the N III $2s^2p^2\,^4P - 2s^2p\,^2P$ multiplet, basically two constraints on Einstein $A$-coefficients may be determined with precision. First, in plasmas which are optically thin in the lines of this multiplet, the ratios of intensities of lines with a common upper level (either the $J = 1/2$ or $J = 3/2$ level) are sensitive only to the ratios of the transition probabilities. Second, in plasmas where the electron density is sufficiently high that collisional rates dominate over radiative rates (this occurs when the radiation fields are weak and the electron densities exceed $\sim 10^{11}$ cm$^{-3}$), the upper level population ratios approach Boltzmann values. Since most plasmas where the N III lines are seen in emission have electron temperatures such that $kT_e$ greatly exceeds the fine-structure splitting of the $^4P$ term, this means that the population ratios approach the level degeneracy $g$ and the line intensities for all lines in the multiplet approach $gA$. 

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4.1. IUE Data for N III

We have examined the literature and searched the IUE merged log to identify high-dispersion (echelle) spectra of objects with reliable emission-line fluxes in the N III] 2s2p¹⁴P → 2s2p¹⁰P multiplet. To our knowledge, no useful data are available for main-sequence or more evolved stars. The lines of N III] are, however, prominent in IUE spectra of lower density objects which are photoionized. After examining archival spectra of various objects we identified two with relatively high quality data: RR Tel and V1016 Cyg. We estimate that, on the basis of the work of Lenz & Ayres (1992), we can determine well-exposed relative line fluxes $|F_λ/dλ|$ to approximately ±5% and 10%, translating to uncertainties in line ratios of ±7% and ±14%, for RR Tel and V1016 Cyg, respectively. The largest single source of uncertainty lies in unknown blended lines.

Figure 1 shows our co-added and filtered IUE spectra for RR Tel (images SWP20251, 10 minute exposure; SWP20247, 20 minutes; SWP22531, 40 minutes; SWP29535, 220 minutes) and V1016 Cyg (images SWP13432, 150 minutes; SWP13705, 60 minutes; SWP16700, 330 minutes through the small aperture, fluxes scaled up by a factor of 2). These data were reduced following the procedure described by Judge & Jordan (1991). The RR Tel line flux spectrum has decayed in time; our co-addition procedure therefore must be checked for systematic errors since the N III region contains saturated pixels in the $λ\lambda1749.674$ and 1752.160 lines which are replaced by “good” pixels from the earlier images. Comparisons of the weaker lines ($λ\lambda1748.674$ and 1753.986), both well exposed in images SWP22531 and SWP29535, indicate that, at worst, we probably overestimate the integrated flux in the $λ1749$ relative to the other lines by less than 3%. This is smaller than the other sources of error, and so we have neglected it.

Unfortunately, we have to criticize work by Keenan et al. (1994) on several grounds. First, they used data for RR Tel from image SWP29535 in which two of the three lines are saturated (see Fig. 1). Our co-addition of data filtered out these saturated data, replacing bad pixels with good ones to produce the best quality spectrum possible. Second, all of their ratios were taken with regard to the line at 1749.674 Å, which is the most badly saturated line in image SWP29535. Third, and related, they do not discuss uncertainties in their data. Fourth, their analysis used radiative data from Stafford et al. (1993), theoretical data now known to be in error (Bell et al. 1994). Fifth, they did not attempt to assign error bars on derived densities $Δ\log N_e$ from errors in flux ratios $ΔR_e$. The derivative terms $d\log N_e/dR_e$ are extremely large for plasmas with $N_e$ in the range $10^5$–$10^6$ cm$^{-3}$. These densities are in the range of the densities they derived for their plasmas.

4.2. Solar Data for N III

Existing solar data have several problems: (1) The disk spectrum at 1750 Å is dominated by strong continuum formed in the upper photosphere; we are therefore limited to spectra obtained above the solar limb. (2) There are problems with blended lines (see below). (3) The largest data set is from the SO82B instrument on Skylab, which, because film was used as a detector, is limited in photometric precision. This is a pity because off-limb data from the active Sun offer us a regime at high enough density that the line emissivities depend primarily on oscillator strengths (and not collision rates). No data from the ultraviolet spectrometer and polarimeter (UVSP) instrument on the Solar Maximum Mission (SMM) satellite are suitable (J. Gurman 1994, private communication).

Nevertheless, we have investigated data from two sources, Doschek et al. (1976) and Sandlin, Brueckner, & Tousey (1977), who studied quiet and active regions, respectively. Both used photographic spectra from the SO82B spectrograph on Skylab, with the slit positioned above the solar limb. We used data tabulated at 4" above the limb in both cases. The relative
photometric precision of these Skylab data is uncertain, but for well-exposed lines of comparable intensity it may be as good as ±7%. We adopt conservative errors of ±20% for ratios of the N III lines tabulated by these authors, on the basis of the spread of points in the photographic density/intensity curves for Skylab (e.g., Doschek et al. 1976).

Table 5 lists our adopted measurements of lines in these data sets.

### 4.3. Analysis of Observed Line Ratios

#### 4.3.1. Lines Sharing Common Upper Levels

Figure 2 shows two sets of line ratios. The left panel shows ratios of lines which share a common upper level and which therefore should primarily reflect the ratios of transition probabilities. The right panel shows the remaining three ratios whose intensities are sensitive to the electron density of the plasma through the interplay between radiative decays and collisional de-excitation of the various levels. (In the nomenclature of Judge et al. 1992, the left panel shows ratios $R_4 = I_{1746.822}/I_{1746.822}$ and $R_5 = I_{1752.160}/I_{1752.160}$, and the right panel shows ratios $R_4 = I_{1749.646}/I_{1753.986}$, $R_2 = I_{1749.646}/I_{1752.160}$, and $R_3 = I_{1749.646}/I_{1752.160}$.)

To within observational uncertainties, observed ratios $R_5$ are in agreement with the theoretical values, given the fact that there is evidence (below) that the $\lambda 1748.646$ line is blended with a line or camera artifact at longer wavelengths in RR Tel (near 1748.8 Å; Fig. 1). Ratio $R_4$, which has large uncertainties owing to the weakness of $\lambda 1746.822$, shows a systematic effect: in RR Tel and V1016 Cyg the ratio is in good agreement with the theoretical value, but in the Sun the ratio is too small by a factor of 10 or more, due to blends (see below).

From these comparisons we infer the following: (1) to within observational uncertainties the theoretical branching ratios determining $R_4$ and $R_3$ are correct to typically ±10%, and (2) the solar ratio $R_4$ (but probably not $R_3$) is influenced by blends (e.g., Feldman & Doschek 1979). Since the lines are optically thin (even at the solar limb), the anomalous solar line ratios

| TABLE 5 |
| --- | --- | --- | --- | --- |
| **Measured Relative Fluxes and Intensities** |
| **OBJECT** | $I(\lambda 1749.674)$ | $\lambda 1746.822$ | $\lambda 1748.646$ | $\lambda 1749.674$ | $\lambda 1752.160$ | $\lambda 1753.986$ |
| **Relative Intensity** | 1.0 | 29 | 21 | 100 | 16 | 21 |
| **Uncertainty (%)** | 15 | 30 | 15 | 5 | 5 |
| **Notes** | All numbers are normalized to the $\lambda 1749.674$ line. For the Sun, only relative intensities are given. For the IUE data, $I(1749.674)$ is in units of $10^{-15}$ ergs cm$^{-2}$ s$^{-1}$. |
most likely result from the anomalous strength of $\lambda 1746.822$, and not the weakness of $\lambda 1752.160$. A search through the listing of Kelly (1987) and through a list of lines generated from an updated list of levels of Fe II (S. Johansson 1989, private communication) has led us to agree with Burton & Ridgeley (1970): the blend is due to a line of Fe II multiplet UV101 ($\lambda 1746.816$, $3d^7 a^2 G_{9/2} \rightarrow 3d^7 l^2 G_{9/2}$) (Moore 1950). The other strong line of multiplet UV101 ($\lambda 1761.372$, with the $J = 7/2$ upper level) is present at roughly the same intensity as the measured feature at $\lambda 1746.82$ (Doschek et al. 1976). Therefore, the measured solar feature at $\lambda 1746.82$ is consistent with its being mostly due to Fe II UV101.

Additional evidence in support of the influence of Fe II UV101 may be found in a different situation in RR Tel's spectrum. In this spectrum, $\alpha 1761.372$ line is absent, but a previously unidentified line is seen (Penston et al. 1983) at 2522.90 Å, which could arise from a line sharing a common upper level ($\lambda 2522.892$, $e^2 G_{9/2} \rightarrow w^2 G_{9/2}$) which, according to Kurucz (1988), has an Einstein $A$-value comparable to that of the $\lambda 1746.816$ line. In RR Tel, it is likely that this line is, in fact, photoexcited by the blended N III line, since lines from the $w^2 G_{7/2}$ level are absent. (A previous example of a weak transition exciting a stronger transition was discussed by Judge, Carpenter, & Harper 1991, where permitted lines of Ni II are excited by intersystem lines of Si II). Therefore, the plotted ratio $R_5$ for RR Tel must be considered a lower limit.

From Figure 2, we suggest that neither of the two lines of $R_5$ at 1753.986, 1748.646 Å are strongly blended, since otherwise dominant blends would have to be of nearly equal intensities so as to produce an accidental agreement between theory and observation in Figure 2.

Doschek et al. (1976) indicate that the observed feature at 1752.12 Å is blended with a line (unspecified by them) and is therefore not totally due to N III $\lambda 1752.160$. Sandlin et al. (1977) could find no reason to suspect blending (their measured wavelength was $1752.14 \pm 0.01$ Å). They also are unable to find a suitable candidate for blending. Certainly, no line between known levels of Fe II can be responsible.

To summarize the issues concerning blended lines: the weakest line ($\lambda 1746.646$) is strongly blended in solar data, and in RR Tel we suspect that a fluorescent excitation of an Fe II line at 2522.892 Å, occurs (this may be checked in future by searching for a weaker line of a common upper level at 2525.114 Å with the GHR5). We conclude that blends in lines $\lambda 1753.986$ and 1748.646 are likely to be small in all our data, with $\lambda 1746.646$ blended with an unknown emission line or artifact close to 1748.8 Å in RR Tel, and it is not possible to judge the quality of the remaining lines.

### 4.3.2. Density-sensitive Lines from Different Upper Levels

Of the data sets under study, the active region data of Sandlin et al. (1977) are the most likely to be representative of conditions where populations are close to Boltzmann ratios. The right-hand panel of Figure 2 shows observed ratios plotted together with calculations of line intensities using collisional data from Blum & Pradhan (1992), the oscillator strengths listed in Table 4, and oscillator strengths for the $^4 P_{1/2}$ level adjusted so as to agree with the measured lifetime, as a func-
tation of electron density. Electron densities are from sources listed by Judge et al. (1993), except for the “active Sun” for which the electron density is simply set to twice that of the quiet Sun (this does not influence our conclusions). The large error bars on the solar data show that we are unable to discriminate between the theoretical and measured Einstein A-coefficients, even if we could determine the electron density accurately for a given plasma. What is needed are high signal-to-noise data for a plasma where the electron density is known to be greater than $10^{11}$ cm$^{-3}$. Solar active region data above the limb (or perhaps during a flare on the disk) would be very valuable. Unfortunately, no instrument we are aware of is scheduled to observe this spectral region. Alternatively, medium-resolution GHRS observations of an active, cool dwarf star may provide additional useful data.

It is interesting to compare the RR Tel and V1016 Cyg data to the theoretical ratios. In the regime where electron densities are in the neighborhood of $10^7$ cm$^{-3}$, these line ratios are controlled by the ratio of the sum of collision strengths from both of the $^2P_0$ levels to the individual $^4P_J$ levels and the radiative branching ratios:

$$ R_1(\text{lim } N_e \to 10^6 \text{ cm}^{-3}) \sim \frac{Y_3}{Y_2} \frac{A_{31} + A_{32}}{A_{32}}, $$

$$ R_2(\text{lim } N_e \to 10^6 \text{ cm}^{-3}) \sim \frac{Y_4}{Y_3} \frac{A_{41} + A_{42}}{A_{42}}, $$

$$ R_3(\text{lim } N_e \to 10^6 \text{ cm}^{-3}) \sim \frac{Y_3}{Y_4} \frac{A_{32} + A_{31} + A_{32}}{A_{42}}, $$

where the subscripts on the right-hand sides of these relations label the atomic energy levels in order of ascending energy (1 = $^2P_{1/2}$, 2 = $^2P_{3/2}$, etc.), and we have used the notation $Y_i$ for the summed Maxwellian-averaged collision strength from levels 1 and 2 to level i, and the $A_i$s are Einstein A-coefficients.

If the branching ratios [e.g., $A_{32}/(A_{31} + A_{32})$] are accurate, as we claim above, and the lines are formed in plasmas where $N_e$ is less than $10^8$ cm$^{-3}$ (this contrast with the conclusions of Keenan et al. 1994), then the only terms left influencing the line ratios $R$ in the regime of interest in RR Tel and V1016 Cyg are ratios of the parameters $Y$. Inspection of these equations and the figure suggests several possibilities, the simplest of which is that the value of $Y_4$ (i.e., the total collision strength to the $^4P_{3/2}$ level) computed by Blum & Pradhan (1992) has been underestimated by a factor of 1.5, relative to $Y_3$ and $Y_5$. Alternative explanations would seem to require invoking inversions in margin of the lines, since, even if the lines are formed in higher density plasmas, as suggested by Keenan et al. (1994), no self-consistent single density can account for all three lines simultaneously.

5. CONCLUSIONS

We have used the ab initio MCHF method to compute oscillator strengths for allowed transitions and, more important, rates for inter system lines of Ni II. We estimate the uncertainty of the latter to be $\sim 5\%$, judging from the different criteria we can use. The deviation from the experimental lifetime of the $^4P_{1/2}$ cannot be explained. Further investigations of this system are therefore warranted. Comparisons with existing spectra of astronomical objects including the Sun cannot provide an answer to the discrepancy, but they do confirm the reliability of our calculated branching ratios at a level of $\pm 10\%$. We have made suggestions for future solar and stellar observations which may help to clarify the situation.

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