NON-LTE EQUIVALENT WIDTHS FOR Ne I WITH ERROR ESTIMATES

T. A. A. SIGUT

Department of Physics and Astronomy, The University of Western Ontario, London, Ontario N6A 3K7, Canada

Received 1998 October 5; accepted 1999 February 3

ABSTRACT

Non-LTE equivalent widths for the $3s \rightarrow 3p$ transitions of Ne I are presented. These lines, which are the strongest available for determining neon abundances in late- to mid-B stars, are known to be subject to large non-LTE strengthening. Error bounds on the equivalent widths arising from uncertainties in the atomic data are evaluated through Monte Carlo simulation, and the non-LTE predictions are explicitly shown to have converged with respect to further increases in model atom complexity. The results are obtainable as a grid of equivalent widths and theoretical uncertainties spanning the entire main-sequence range of B star stellar parameters ($T_{\text{eff}} = 10,000$–$31,000$ K, log $g = 3.5$–$4.5$, and $\zeta_r = 0$–$10$ km s$^{-1}$) for three choices of the neon abundance ($A_{\text{Ne}} = 7.55$, 8.05, and 8.55 dex). Over most of this range, for realistic observing programs and using currently available atomic data, the limiting accuracy of neon abundance determinations based on Ne I is $\pm 0.10$ dex.

Subject headings: radiative transfer — stars: abundances — stars: mass loss

1. INTRODUCTION: MOTIVATION FOR ACCURATE NEON ABUNDANCES

The nucleosynthesis of neon proceeds through the $x$-sequence of nuclear reactions, and as such the abundance of neon in a variety of astrophysical objects is an important test of the theory of stellar evolution. Sampling neon abundances at a range of positions in the Galactic disk helps to reconstruct the nucleosynthesis history of our Galaxy. Galactic abundance gradients in neon are well established for H II regions (Simpson et al. 1995) and planetary nebulae (Maciel & Köppen 1994). In addition, neon is one of the few elements for which an abundance gradient with Galactocentric distance is detected using early B stars in open clusters, as based on the LTE analysis of Ne II (Kilian-Montenbruck, Gehren, & Nissen 1994).

An accurate value for the solar photospheric neon abundance is difficult to obtain. No photospheric lines of Ne I are available because of the high energies of the lowest excited states, and CI meteorites fail to provide data for noble gases. The solar corona, solar wind, and solar energetic particles all provide observed neon abundances, but their relationship to a photospheric/meteoritic abundance is complicated by the first ionization potential (FIP) effect, in which there is a large depletion of elements with high FIPs (IP $\gtrsim$ 11 eV) in the solar corona and wind (Grevesse & Anders 1992). A "photospheric" solar neon abundance is obtained either by assuming the average neon abundance derived from other objects in the local Galactic environment, most notably from the Ne/O ratios of nearby H II regions (Meyer 1989), or the solar coronal, wind, and particle measurements are corrected by a FIP depletion factor extrapolated from those of other more reliably determined depleted elements such as carbon, nitrogen, and oxygen. Both estimates are in reasonable agreement, giving $A_{\text{Ne}} \equiv \log_{10} (N_{\text{Ne}}/N_{\text{H}}) + 12 = 8.09 \pm 0.1$ dex (Grevesse & Anders 1992), although some discordant data do exist (Meyer 1989). Thus neon abundances derived from objects in the local Galactic environment affect the estimate of the solar neon abundance in a fundamental way. Stellar abundances could potentially play an important role in this determination, but, for reasons discussed below, reliable abundances from the analysis of the Ne I spectrum have been difficult to obtain.

Central to the motivation of the present work, however, is the possibility that accurate neon abundances may allow the detection of weak stellar winds in late- to mid-B stars. Such winds seem required by diffusion theory in order to explain many chemical peculiarities among the upper main sequence (such as helium overabundances), but, because the required mass-loss rates are only $\sim 10^{-14}$ to $10^{-12}$ $M_\odot$ yr$^{-1}$, they are exceedingly difficult to detect by conventional means such as line asymmetries. The single example of the detection of such a weak stellar wind is by Bertin et al. (1995), who claim a mass loss from $\sim 2 \times 10^{-13}$ to $1.5 \times 10^{-12}$ $M_\odot$ yr$^{-1}$ from Sirius (A1 V) from the analysis of extremely weak absorption features in the resonance lines of Mg II and H I. Recently, Landstreet, Dolez, & Vauclair (1998) have argued that overabundances of neon and oxygen, not predicted by conventional diffusion theory because of their naturally high cosmic abundances, may result from the combined action of diffusion and a weak stellar wind, and thus neon and oxygen abundance may serve as sensitive tracers of this process. Because of the different ionization potentials of their neutral stages, photospheric neon and oxygen abundance are sensitive to weak winds at different $T_{\text{eff}}$, with oxygen being useful in the A to late B range, $T_{\text{eff}} = 8500$–$11,000$ K, whereas neon is useful in the late- to mid-B range, 11,000–16,000 K. Landstreet et al. reach no definite conclusion as to the presence of weak stellar winds among the late- and mid-B stars because of the extreme paucity of reliable neon abundances for these objects. Thus the interesting question of whether neon abundance traces weak stellar winds can only be answered by a new systematic study of B star neon abundances, which requires accurate non-LTE calculations over the required range of stellar parameters.

2. CALCULATIONS

Determining accurate neon abundances from stellar spectra is a challenging problem. The high excitation energies of even the lowest Ne I excited states means that lines useful for abundance determinations become first detectable only in late B stars ($T_{\text{eff}} \gtrsim 11,000$ K) and are typically
quite weak ($W_s \ll 50 \text{ mÅ}$). In addition, all of the Ne I lines used for abundance analysis are known to be subject to large non-LTE strengthening. Observed neon abundances in early-type stars were a complete puzzle, being much too large compared to other objects such as H II regions and planetary nebulae, until the pioneering work of Auer & Mihalas (1973b). They demonstrated that even though the Ne I spectrum is weak, large non-LTE effects are still present, which result in enhancements of the equivalent widths in the $3s \rightarrow 3p$ transition array by factors approaching 2.

The range of stellar parameters that define the current computational grid are listed in Table 1. At each point, defined by effective temperature, $T_{\text{eff}}$, surface gravity, log $g$, microturbulence, $\zeta$, and neon abundance, $A_{\text{Ne}}$, non-LTE solutions were obtained for 30 Ne I atomic models that were randomly realized from the estimated error distributions of the default atomic data (see § 2.1). By using the same set of atomic models for each point in the computational grid, each neon transition is represented by a set of curves of growth that can be used to determine 30 estimates of the neon abundance and microturbulent velocity (determined in the usual way by requiring that the derived abundance be independent of equivalent width). The resulting distributions in $A_{\text{Ne}}$ and $\zeta$ are a measure of the accuracy of these parameters due to uncertainties in the atomic data. This derived accuracy is a limiting accuracy as additional sources of errors, such as improper $T_{\text{eff}}$, log $g$ calibrations, or errors in the observed equivalent widths, are not considered. This technique to assess the reliability of non-LTE equivalent width calculations is further discussed by Sigut (1996).

2.1. Model Atom

All Ne I energy levels for $n \leq 5$ have been included in the model atom, resulting in 37 non-LTE levels. This value ensures that the energy gap left before the Ne II continuum is less than $kT$, a general requirement for determining an accurate ionization fraction for a trace ionization stage (Sigut & Lester 1996). The completeness of the model atom is explicitly investigated below by adding hydrogenic composite levels up to $n = 8$. These additional levels were found to have no influence on the equivalent width predictions in the $3s \rightarrow 3p$ transition array and were not retained for the full calculations. Experimental energies were taken from Moore (1949).

The excited states of Ne I are of the form $2p^5(2P_J)n\ell$ and consist of a weakly bound active electron interacting with a tightly bound atomic core. The resulting energy levels are poorly described by LS coupling and are generally described instead by $j/\ell$ (sometimes called $jK$) coupling as $j, [K^j]$, and $I$, $P$, $F$, $S$, and $J$ are the total angular momentum of the core, $\ell$ or $\frac{1}{2}$ in the case of Ne I; $K$ is the coupling of $j$, with $\ell$; and $J$, the total angular momentum, is the coupling of $K$ with the spin of the active electron. For configurations closely approximated by $j/\ell$ coupling, the latter step gives two closely spaced energy levels, and, as a result, $j/\ell$ coupling is often called pair coupling. A significant complexity, however, is that while the energy levels of Ne I are usually labeled by $j/\ell$ notation, the actual states are often strongly mixed resulting in intermediate coupling; this makes accurate atomic data a more challenging computational problem than in the more familiar case of states well-approximated by $LS$ (or $jK$) coupling.

The fine-structure splitting of the 3s, 3p, and 4s configurations has been retained. The remaining levels for $n \leq 5$ have been summed over $K$, giving levels labeled by $n\ell'$ or $n\ell''$, depending on the value of $j_c$ (primed designating $j_c = \frac{3}{2}$; primed designating $j_c = \frac{1}{2}$). Table 2 lists the included energy levels, and Figure 1 shows a Grotrian diagram for Ne I in which the fine-structure radiative transitions among the 3s, 3p, and 4s levels are shown. Table 2 also gives the original Paschen notation for the energy levels, a labeling scheme adopted in many older works.

Radiative data (oscillator strengths and photoionization cross sections) for Ne I have been computed by the Opacity Project (OP) under the assumption of LS coupling (Hibbert

### TABLE 1

| Parameter          | Range   | Step |
|--------------------|---------|------|
| $T_{\text{eff}}$ (K) | 10000–31000 | 2000 |
| log $g$           | 3.5–4.5 | 0.5  |
| $\zeta$ (km s$^{-1}$)  | 0–10    | 5    |
| $A_{\text{Ne}}$    | 7.55–8.55 | 0.5  |

### TABLE 2

**Ne I Energy Levels**

| Number | $E_i$ (cm$^{-1}$) | $g_i$ | $[K]^n\ell'$ | Paschen |
|--------|------------------|------|--------------|---------|
| 1      | 0.00             | 1    | $2p^53s$     | ...     |
| 2      | 134,041.84       | 5    | $2p^53s$     | $1s_9$  |
| 3      | 134,459.28       | 3    | $2p^53s$     | $1s_8$  |
| 4      | 134,818.64       | 1    | $2p^53s$     | $1s_7$  |
| 5      | 135,885.72       | 3    | $2p^53s'$    | $1s_8$  |
| 6      | 148,257.80       | 3    | $2p^53p$     | $2p_{10}$ |
| 7      | 149,657.05       | 7    | $2p^53p$     | $2p_9$  |
| 8      | 149,824.22       | 5    | $2p^53p$     | $2p_8$  |
| 9      | 150,121.59       | 5    | $2p^53p$     | $2p_7$  |
| 10     | 150,315.86       | 5    | $2p^53p$     | $2p_6$  |
| 11     | 150,772.17       | 3    | $2p^53p$     | $2p_5$  |
| 12     | 150,858.52       | 5    | $2p^53p$     | $2p_4$  |
| 13     | 150,917.44       | 1    | $2p^53p$     | $2p_3$  |
| 14     | 151,038.45       | 3    | $2p^53p$     | $2p_4$  |
| 15     | 152,970.73       | 1    | $2p^53p$     | $2p_4$  |
| 16     | 158,601.11       | 5    | $2p^54s$     | $2s_9$  |
| 17     | 158,706.61       | 3    | $2p^54s$     | $2s_9$  |
| 18     | 159,380.01       | 1    | $2p^54s$     | $2s_9$  |
| 19     | 159,534.62       | 3    | $2p^54s$     | $2s_9$  |
| 20     | 161,262.06       | 40   | 3$d$         | ...     |
| 21     | 162,416.08       | 20   | 3$d$         | ...     |
| 22     | 162,895.62       | 24   | 4$p$         | ...     |
| 23     | 163,743.66       | 12   | 4$p$         | ...     |
| 24     | 165,859.91       | 8    | 5$s$         | ...     |
| 25     | 166,643.97       | 4    | 5$s'$        | ...     |
| 26     | 167,015.48       | 40   | 4$d'$        | ...     |
| 27     | 167,065.86       | 56   | 4$f$         | ...     |
| 28     | 167,593.62       | 24   | 5$p$         | ...     |
| 29     | 167,797.70       | 20   | 4$d'$        | ...     |
| 30     | 167,846.55       | 28   | 4$f'$        | ...     |
| 31     | 168,385.25       | 12   | 5$p'$        | ...     |
| 32     | 168,940.66       | 8    | 6$s$         | ...     |
| 33     | 169,511.78       | 40   | 6$d$         | ...     |
| 34     | 169,540.19       | 128  | 5$f,5g$     | ...     |
| 35     | 169,722.20       | 4    | 6$s'$        | ...     |
| 36     | 170,292.33       | 20   | 5$d$         | ...     |
| 37     | 170,322.23       | 66   | 5$f,5g'$     | ...     |

*Note:* $(n\ell')$ indicates $j_c = \frac{3}{2}$, $(n\ell'')$, $j_c = \frac{1}{2}$. 
However, the application of this data to the actual mixed states of Ne I is not straightforward. Fortunately, Seaton (1998a) has developed a semiaempirical method using the experimental energies, which allows the OP f-values to be recoupled to account for the physical mixed states. He finds excellent agreement of these results with the available experimental values ($\pm 10\%$). Seaton (1998b) provides coefficients for the expansion of the photoionization cross sections for Ne I in terms of the OP cross sections computed under LS coupling for all states with $n = 3$ and 4. Again, the expected accuracy of this data set is $\pm 10\%$. The Coulomb approximation has been employed for the remaining radiative transitions between high-$\ell$ levels, with radial integrals computed following Oertel & Shomo (1968) and angular factors for $\ell'$ coupling computed following Cowan (1981).

Contributions to line broadening included radiative broadening and the pressure broadening of neutral perturbers (van der Waals) and charged perturbers (quadratic Stark). For temperatures and pressures typical of B star photospheres, Stark broadening dominates, and damping widths for this process were computed with the method of Dimitrijević & Konjević (1986). Because the Ne I lines are generally weak, the uncertainty in this approximation (estimated at typically $\pm 50\%$) has a negligible affect on the predicted line strengths. All of the LTE line formation parameters for the $3s \rightarrow 3p$ transitions are listed in Table 3.

For electron impact excitation of the $2p^3 3s$ and $2p^3 3p$ configurations from the ground state, the 31 state semi-relativistic R-matrix calculations of Zeman & Bartschat (1997, hereafter ZB97) have been adopted. They give rates to specific fine-structure levels, and thus the assumption of statistical branching ratios is not made. For the collisional excitation of a few transitions between the $2p^3 3s$ and $2p^3 3p$ configurations, the $R$-matrix results of Taylor, Clark, & Fon (1985, hereafter TCF85) have been adopted. This calculation is performed in LS coupling, and some procedure is required to assign these results to the pair-coupled states and to split the total multiplet strengths among the fine-structure transitions. For collisional transitions between the $2p^3 3s$ levels, the LS strengths have been split according to their statistical weights (see Pradhan & Gallagher 1992) and then assigned according to the scheme $3s(1s_1, 1s_2, 1s_3, 1s_4) \rightarrow 3s(3P^2_2, 3P^2_1, 3P^0_0, 1P^1_1)$. Because the $2p^3 3s$ states are well described by LS coupling (Phillips, Anderson, & Lin 1985), these assignments are meaningful.

The TCF85 LS rates are also used for transitions from $3p^3 P^0$ to $3p^3 1D^0$, $3p^3 1P^0$, and $3p^3 1S^0$. The latter states have been identified with $2p_6, 2p_2$, and $2p_1$, respectively.

For all remaining transitions for which f-values are available, collision strengths were computed using the impact parameter approximation of Seaton (1962). For collision strengths between fine-structure components of total jK states, a unit effective collision strength has been assumed. For remaining transitions without collision strengths, the collision strength has been set to 10% of the nearest allowed collisional transition (in energy) arising from the same lower level. For collisional ionization, the rate was computed using the approximation given by Mihalas (1978, that paper's eq. [5-79]).

For $T_{\text{eff}} < 23,000$ K, Ne II was represented by a single atomic level, and Ne III was not included; for higher $T_{\text{eff}}$, Ne II was represented by 11 bound LS multiplet states [all levels up to and including $2p^4(1P)3p^2 2P^0$], and Ne III was
represented by a single bound level. Experimental energies were taken from Moore (1949). All radiative atomic data were taken from the 1988 OP project calculations of K. Butler and C. J. Zeippen from the TOPBASE database (Cunto et al. 1993). Collision strengths were computed with the effective Gaunt factor formulae of Van Regemorter (1962), despite its known limitations (Sampson & Zhang 1992). Stark broadening parameters for the 10 Ne ii lines were computed with the OP approximation of Seaton (1987, 1988).

This defines the default atomic data set. The expected accuracy of each category of atomic data is given in Table 4. Each atomic parameter in this table is assumed equally well-converged within a scale factor ranging over ± log p, where p is the uncertainty assigned in the table. Because all of the atomic data are from theoretical calculation, the errors are determined by systematic effects due to the approximate methods used, and hence a more complex error distribution function is unwarranted. The uncertainties in the photoionization rates have been increased to reflect uncertainties in the photoionizing radiation field. Larger uncertainties are assigned to the TCF85 collision strengths as based on comparison with the more accurate results of ZB97, the somewhat schematic assignment of the LS rates to pair-coupled levels, and the fact that these rates are to the last bound channels in the calculation and such transitions are generally poorly converged in R-matrix calculations (Sawey et al. 1990). The impact parameter approximation is generally believed to give results accurate to within a factor of 2 for strong radiatively allowed transitions. Comparison of the impact parameter method with the R-matrix results for the seven transitions in common gives results somewhat worse than this, with some transitions differing by a factor of ~ 10. As a result, a value of p = 3.0 is assigned to the impact parameter rates.

Thirty atomic models were randomly realized from the discussed atomic data using uncertainties listed in Table 4. These model atoms were used as the basis for the Ne i equivalent width grid.

### 2.2. Model Atmospheres

The coupled equations of radiative transfer and statistical equilibrium were solved with the MULTI code (Carlsson 1986) in its local operator form (version 2.0, Carlsson 1992). A replacement continuous opacity package was used (Sigut & Lester 1996). The opacity routine is based on the extensive one available in the model atmosphere program ATLAS9 (Kurucz 1992) and is appropriate for early-type stars.

Kurucz, LTE, line-blanketed, model atmospheres were used for the entire range of the computational grid. These models provided not only the basic physical conditions in the stellar photospheres (temperature and pressure) but also the photoionizing radiation fields. The photoionization and

### TABLE 3

**LTE Line Formation Parameters for the 3s → 3p Transitions of Ne i**

| Transition | λ_{air} (Å) | g_i | g_j | f_{ij} | γ_{ion}/N_e | EW | R | R^{AM} |
|------------|-------------|-----|-----|--------|--------------|----|---|--------|
| 3s_{1/2}^+ → 3p_{1/2}^+ | 5852.49 | 3 | 1 | 1.08^{-1} | 7.59^{-6} | 17.0 | 1.51 | 1.8 |
| 3s_{3/2}^+ → 3p_{1/2}^+ | 5881.89 | 5 | 3 | 3.42^{-2} | 5.64^{-6} | 12.7 | 1.70 | 1.9 |
| 3s_{3/2}^+ → 3p_{3/2}^+ | 5944.83 | 5 | 5 | 5.80^{-2} | 5.18^{-6} | 19.9 | 1.69 | 1.9 |
| 2s_{1/2}^+ → 3p_{1/2}^+ | 5975.50 | 5 | 7 | 1.06^{-2} | 5.60^{-6} | 3.9 | 1.55 | 1.7 |
| 2s_{1/2}^+ → 3p_{3/2}^+ | 6074.30 | 3 | 1 | 1.05^{-1} | 6.19^{-6} | 18.7 | 1.59 | 1.8 |
| 2s_{3/2}^+ → 3p_{1/2}^+ | 6096.16 | 3 | 5 | 1.63^{-1} | 5.28^{-6} | 27.9 | 1.64 | ... |
| 2s_{3/2}^+ → 3p_{3/2}^+ | 6143.06 | 5 | 5 | 1.58^{-1} | 5.10^{-6} | 46.7 | 1.84 | 1.9 |
| 3s_{1/2}^+ → 3p_{3/2}^+ | 6163.50 | 1 | 3 | 2.42^{-1} | 5.30^{-6} | 15.8 | 1.79 | 1.6 |
| 3s_{3/2}^+ → 3p_{3/2}^+ | 6217.30 | 5 | 5 | 2.12^{-2} | 5.25^{-6} | 7.6 | 1.70 | 1.8 |
| 3s_{1/2}^+ → 3p_{1/2}^+ | 6266.50 | 1 | 3 | 4.27^{-1} | 5.26^{-6} | 25.0 | 1.77 | 1.8 |
| 3s_{3/2}^+ → 3p_{1/2}^+ | 6334.50 | 5 | 5 | 9.68^{-2} | 4.76^{-6} | 30.0 | 1.80 | 1.9 |
| 3s_{3/2}^+ → 3p_{3/2}^+ | 6383.00 | 3 | 3 | 1.94^{-1} | 5.36^{-6} | 31.0 | 1.69 | 1.8 |
| 2s_{1/2}^+ → 3p_{3/2}^+ | 6402.20 | 5 | 7 | 4.20^{-1} | 4.17^{-6} | 85.5 | 1.80 | 1.8 |
| 2s_{3/2}^+ → 3p_{3/2}^+ | 6506.50 | 3 | 5 | 3.09^{-1} | 4.86^{-6} | 44.2 | 1.74 | 1.9 |
| 3s_{1/2}^+ → 3p_{3/2}^+ | 6598.90 | 3 | 3 | 1.47^{-1} | 5.87^{-6} | 20.9 | 1.78 | 1.7 |
| 3s_{3/2}^+ → 3p_{1/2}^+ | 6678.28 | 3 | 5 | 2.59^{-1} | 5.42^{-6} | 33.5 | 1.73 | ... |
| 3s_{3/2}^+ → 3p_{3/2}^+ | 6717.04 | 3 | 3 | 1.47^{-1} | 5.84^{-6} | 20.3 | 1.70 | ... |
| 3s_{1/2}^+ → 3p_{3/2}^+ | 6929.47 | 3 | 5 | 2.11^{-1} | 5.35^{-6} | 29.4 | 1.89 | ... |

**Note.** Oscillator strengths are from Seaton 1998a; γ_{ion} is the Stark (half) half-width in circular frequency units at T = 10^8 K. EW is the non-LTE equivalent width in mA, tabulated for T_{eff} = 17000 K, log g = 4.0, v = 5 km s^{-1}, and the solar neon abundance (A_ne = 8.05). R is the ratio of the non-LTE to LTE equivalent widths, and the last column gives R as predicted by Auer & Mihalas 1973b for the same stellar parameters. The ratios listed for the current work are for the default atomic data.

### TABLE 4

**Adopted Uncertainties for the Ne i Atomic Data**

| Atomic Parameter | Uncertainty (p) |
|------------------|-----------------|
| f_{ij} (Seaton 1998a) | 1.10 |
| σ_{ion} (Seaton 1998b) | 1.20 |
| Q_{exc}-R matrix, ZB97 | 1.25 |
| Q_{exc}-R matrix, TCF85 | 1.50 |
| Q_{exc}-impact parameter | 3.00 |
| Q_{exc}-ad hoc | 10.00 |
| Q_{ion} | 3.00 |
| γ_{ion} | 1.50 |

**Note.** The atomic parameters are oscillator strength (f_{ij}), photoionization cross section (σ_{ion}), collision strength (Q_{exc}) for excitation/ionization, and Stark damping width (γ_{ion}).
stimulated recombination rates were computed using the ATLAS9 high-resolution opacity distribution function mean intensities, which divide the spectrum into 1221 frequency bins of widths ~ 10 Å. The use of LTE model atmospheres is discussed and justified for this range of stellar parameters by Sigut & Lester (1996) and Sigut (1996). Because the focus of this calculation is on the late- to mid-B stars, the use of LTE model atmospheres should not introduce large uncertainties into the calculation (see also Grigsby, Morrison, & Anderson 1992).

3. RESULTS

3.1. Non-LTE Effects in Ne I

Departure coefficients\(^1\) for Ne I are shown in Figure 2 at \(T_{\text{eff}} = 17,000\) K and \(\log g = 4.0\). For \(\log \tau_{5000} \geq -0.5\), all levels closely follow their LTE populations, but at smaller optical depths the ground state and \(2p^5 3s\) levels become overpopulated with respect to the \(2p^5 3p\) levels, with the latter remaining at nearly their LTE populations. Despite the small departures from LTE exhibited by the level populations, there are large enhancements in the strengths of the \(3s \rightarrow 3p\) transitions. For example, Figure 3 shows the equivalent width of \(\lambda 6402\), the strongest Ne I transition, for three choices of the neon abundance. The 30 curves shown for each abundance correspond to the 30 Monte Carlo simulations. There is a large non-LTE strengthening of the line at all \(T_{\text{eff}}\) and a significant spread in the equivalent widths predicted by the different, but equally probable, atomic models. For example, at maximum strength and for the solar neon abundance \((A_{\text{Ne}} = 8.05)\), equivalent widths range from 70 to 95 mA. Ratios of non-LTE to LTE equivalent widths at \(T_{\text{eff}} = 17,000\) K, \(\log g = 4.0\) for all \(18\) \(3s \rightarrow 3p\) transitions are given in Table 3. Large enhancements are predicted with ratios ranging from 1.51 to 1.81. Table 3 also gives the non-LTE to LTE equivalent width ratios of Auer & Mihalas (1973b) for the same stellar parameters; their ratios are generally comparable to the current results, although there are detailed differences. Figure 3 also shows the LTE equivalent widths for \(\lambda 6402\), demonstrating that there is essentially no \(T_{\text{eff}}\) at which an LTE analysis of the line strengths can be applied. Note the fortuitous agreement of the LTE line strengths for \(A_{\text{Ne}} = 8.55\) with the non-LTE line strengths for \(A_{\text{Ne}} = 8.05\); sizable errors in abundances result from an LTE analysis of the Ne I spectrum.

The inset in Figure 2 shows the predicted Ne I and Ne II ionization fractions. A slight underionization of Ne I, with respect to LTE, in the line-forming regions is shown. Auer & Mihalas (1973b) attribute the strong non-LTE strengthening of the \(3s \rightarrow 3p\) transitions to amplification of the small non-LTE departures by the stimulated emission correction to the line source function. Consider a line transition \(l \rightarrow u\) with frequency \(v\), and let \(\delta = hv/kT\) and \(\beta_l/\beta_u = 1 + \epsilon\). The ratio of the line source function to the Planck function is

\[
\frac{S_{lu}}{B_l(T)} = \frac{e^\delta - 1}{(1 + \epsilon)e^\delta - 1}. \tag{1}
\]

If stimulated emission is negligible, then

\[
\frac{S_{lu}}{B_l(T)} \sim (1 + \epsilon)^{-1}, \tag{2}
\]

whereas if stimulated emission is important \((\delta \ll 1)\),

\[
\frac{S_{lu}}{B_l(T)} \sim \left(1 + \frac{\epsilon}{\delta}\right)^{-1}. \tag{3}
\]

Hence, if stimulated emission is important, the line source function can be vulnerable to small deviations from LTE in

![Fig. 2.—Ne I departure coefficients near the maximum strength of the \(3s \rightarrow 3p\) transitions at \(T_{\text{eff}} = 17,000\) K, \(\log g = 4.0\), \(\zeta = 5\) km s\(^{-1}\), and \(A_{\text{Ne}} = 8.05\). The line styles indicate different levels in the Ne I atom. The inset shows the ionization fractions of Ne I and Ne II relative to LTE.](image-url)
the level populations: a given deviation from LTE in the population ratio is amplified by a factor of $\delta$. Auer & Mihalas (1973a) invoke this mechanism to explain the large non-LTE enhancements of the red lines of He ii in early B stars.

However, the current non-LTE calculation does not identify this mechanism as the critical factor in the large non-LTE corrections. First, the stimulated emission correction for the red Ne i lines is not that large ($\delta$ is not $\ll 1$); for $\lambda = 6000$ Å, $e^{\nu k T} = e^{k T}$, where $T_e$ is the temperature in units of $10^4$ K. Hence, over the relevant temperature range, amplification of the deviations of $B_i/B_u$ from unity does not occur. This is demonstrated in the left panel of Figure 4, where the line source function for $\lambda 6402$ at $T_{\text{eff}} = 17,000$ K, log $g = 4.0$ is shown with and without the correction for stimulated emission. There is little difference between the two predictions, and a significant non-LTE strengthening of the line would result even if the stimulated emission correction to the line source function were ignored. The depth of formation of the emergent line flux for 0–4 Doppler widths from line center is also shown using the contribution function proposed by Achmad, de Jager, & Nieuwenhuijzen (1991). The line flux at line center is seen to form at log $\tau_{5000} \sim -1.3$, precisely in the region where $S_u/B_s(T) < 1$, leading to an increase in the line depth.

A more subtle aspect of the limit $\delta \ll 1$ is that the departure coefficients of the upper and lower levels of a transition can be controlled by rates other than the radiative and collisional rates directly between the two levels. Coupling to other levels can result in dramatic non-LTE effects, such as the Mg i 12 µm emission lines in the solar spectrum (Carlsson, Rutten, & Shchukina 1992; see also Sigut & Lester 1996 for a discussion of this point). However, in the current case, the dominant rates controlling the overpopulation of the 3s levels are found to be the radiative and collisional rates within the 3s $\to$ 3p transition array. To demonstrate this point, a multi-MULTI analysis (Carlsson et al. 1992) was performed in which each radiative and collisional rate in the default atomic model was increased, in turn, by a factor of 2, and then the non-LTE solution converged, a procedure resulting in 877 individual non-LTE runs. For each radiative transition, a list of the most influencial rates, rates whose doubling resulted in the largest changes to the equivalent width, can be compiled. The results of such a multi-MULTI analysis for $\lambda 6402$ are summarized in Table 5. Aside from its own oscillator strength, this transition is most sensitive to its own collision strength, showing a $\sim 10\%$ weakening for a factor of 2 increase in the collision strength as the line source function is brought

| Change (%) | $i$ | $j$ | Type | Transition |
|------------|----|----|------|------------|
| + 55.16     | 2  | 7  | rbb  | [3/2]3s $\to$ [3/2]3p |
| - 8.54      | 2  | 7  | cbb  | [3/2]3s $\to$ [3/2]3p |
| + 1.15      | 2  | 10 | rbb  | [3/2]3s $\to$ [3/2]3p |
| - 0.99      | 1  | 38 | rbb  | 2p^6(He i) $\to$ 2p^5(He ii) |
| + 0.89      | 2  | 8  | rbb  | [3/2]3s $\to$ [3/2]3p |
| - 0.88      | 2  | 8  | cbb  | [3/2]3s $\to$ [3/2]3p |
| - 0.87      | 2  | 6  | cbb  | [3/2]3s $\to$ [3/2]3p |
| + 0.80      | 2  | 6  | rbb  | [3/2]3s $\to$ [3/2]3p |
| - 0.71      | 7  | 20 | rbb  | [3/2]3p $\to$ 3d |
| - 0.60      | 2  | 5  | cbb  | [3/2]3s $\to$ [3/2]3p |

Note.—Rate types are identified as rbb (radiative bound-bound), rbf (radiative bound-free), and cbb (collisional bound-bound) transitions.
closer to the local Planck function in the line-forming regions. The remaining influential rates generally correspond to other radiative and collision transitions between levels of the 3s and 3p configurations.

In conclusion, the lines of the 3s → 3p transition array are dominated by the classic non-LTE effect of photons losses in the line(s) leading to an overpopulation of the lower level(s). The line source function drops below the local Planck function, leading naturally to stronger lines. The fact that the lines are in the red region of the spectrum is important in that there is a larger continuous opacity, which forces the depth of formation of the lines to smaller optical depths where the source function is lower, and that the lines are in the red region of the spectrum is important when a minor ionization stage is coupled to a large LTE reservoir such as the ground state of its parent ion. Roughly, this requires inclusion of levels to principal quantum number where is the effective temperature in units of \(10^4\) K and \(Z\) is the charge, \(Z = 1\) for neutrals, and so on. As expected, in the case of Ne I no significant differences (<2%) were found between the predictions of the \(n = 5\) and \(n = 8\) atomic models over the entire range of stellar parameters. Hence the smaller atomic model was retained for the calculation.

3.3. Limiting Accuracy of Neon Abundances

Table 6 gives the predicted equivalent widths for the strongest Ne I transition, \(\lambda 6402\), for a range of stellar parameters and neon abundances. Also listed for each equivalent width is the \(2\sigma\) uncertainty as determined by Monte Carlo simulation. Generally, the atomic data uncertainties of Table 4 translate into equivalent width predictions accurate to 10%–20%. Because it is not possible to present the entire grid of equivalent widths for all 18 transitions of Table 3, the full equivalent width grid can be obtained from the author upon request. Note that in order to fully utilize these results, the individual curves of growth for each transition are required, as will now be discussed.
To determine the accuracy of neon abundance determinations based on Ne I due to limitations in the atomic data, the equivalent width grid has been used to derive neon abundances from the predicted equivalent widths for the default atomic model corresponding to $A_{\text{Ne}} = 8.05$ and $\zeta_t = 5 \text{ km s}^{-1}$. Thirty abundance estimates were obtained for each line based on the 30 curves of growth available from the Monte Carlo simulations. This procedure is illustrated in Figure 5, where 100 curves of growth for $\lambda 6402$ are shown at $T_{\text{eff}} = 17,000$ K, $\log g = 4.0$. The larger number of Monte Carlo simulations used is simply for illustration in this example and the one below; these calculations were carried out separately from the main grid. The spread in these curves is entirely due to uncertainties in the atomic data, with all curves being equally probable. This figure illustrates that even in the case of a perfectly accurate observation, there is still a finite uncertainty in the abundance. For example, in this case, an observed equivalent width of 85.5 mÅ translates into abundances ranging from 7.95 to 8.22 dex.

In assessing the overall limiting accuracy of neon abundance determinations, abundances were determined for $T_{\text{eff}} = 17,000$ K, $\log g = 4.0$, 100 curves of growth corresponding to 100 random realizations of the atomic data. Because of uncertainties in the atomic data alone, an infinitely accurate observation (say, 85.5 mÅ) translates into a range of possible abundances ($A_{\text{Ne}} = 7.95–8.22$ dex).

![Figure 5](image-url)
three sets of lines, the first set being the ideal case of all 18 lines of Table 3; a second, more realistic set consisting of four lines, $\lambda\lambda 6143, 6163, 6382$, and 6402; and a final minimal set consisting of only two lines, $\lambda\lambda 6382$ and 6402. The microturbulence was determined simultaneously in the usual way by requiring that the derived abundance be independent of equivalent width. A specific illustration of the resultant distributions of neon abundance and microturbulence estimates obtained is given by the histograms of Figure 6, which are based on 100 Monte Carlo simulations at $T_{\text{eff}} = 17,000$ K, log $g = 4.0$ with all 18 lines of Table 3 used. For perfect observations, the uncertainty in the derived abundance is small, with a value of $8.07 \pm 0.04$ dex recovered. Note, however, the large spread in the derived value for $\zeta_t$ with $5.0 \pm 3.0$ km s$^{-1}$ recovered. Although the mostly weak lines of Ne I are not ideal for microturbulence determinations, the influence of atomic data uncertainties on microturbulence estimates should be borne in mind, in addition to the other sources of uncertainty.

Table 7 gives a summary of limiting accuracies of neon abundance determinations based on Ne I for a range of $T_{\text{eff}}$ and log $g = 4.0$ using the equivalent width grid based on 30 Monte Carlo simulations. Even in the minimal case in which only two lines are used in the analysis, accuracies of $\pm 0.10$ dex are still recovered. However, these limiting precisions reflect only uncertainties due to the atomic data and not, for example, errors in the observed equivalent widths or in the $T_{\text{eff}}$ and log $g$ calibration.

One feature of the abundance distributions that requires comment is that they generally do not recover the input abundance of 8.05 dex within the uncertainty in the mean. For example, in Figure 6 the recovered mean abundance is $8.072 \pm 0.008$. This systematic shift is caused by the input distribution of scalings; each atomic parameter is scaled by factors uniformly probable within $\pm \log p$, where $p$ is taken from Table 4. This ensures that the mean of the scalings is 1, but the nonlinear dependence of the predicted equivalent widths on the atomic rates generally means that the equivalent widths averaged over the 30 Monte Carlo simulations do not exactly recover the unit scaling predictions. However, because it is the widths of the distributions that are of interest, this point is not significant to the current analysis.

### Table 7

| $T_{\text{eff}}$ (K) | Limiting Accuracy (dex) |
|----------------------|-------------------------|
| 10,000...            | 0.028                   |
| 12,000...            | 0.030                   |
| 15,000...            | 0.032                   |
| 17,000...            | 0.032                   |
| 19,000...            | 0.032                   |
| 21,000...            | 0.038                   |
| 23,000...            | 0.038                   |
| 25,000...            | 0.038                   |
| 27,000...            | 0.042                   |
| 29,000...            | 0.048                   |

| 18 Lines | 4 Lines | 2 Lines |
|---------|---------|---------|
| 0.058   | 0.066   | 0.098   |
| 0.074   | 0.072   | 0.108   |
| 0.068   | 0.068   | 0.094   |
| 0.062   | 0.060   | 0.086   |
| 0.060   | 0.060   | 0.086   |

**Note:**—log $g = 4.0$ for all models. The quoted uncertainties are 2 $. The lines included in the three cases are (1) 18 lines, all lines of Table 3, (2) four lines, $\lambda\lambda 6143, 6163, 6382, 6402$, and (3) two lines, $\lambda\lambda 6382, 6402$.

### Figure 6

**Figure 6.**—Histograms showing 100 neon abundance (top) and microturbulence ($\zeta_t$, bottom) determinations at $T_{\text{eff}} = 17,000$ K, log $g = 4.0$, using equivalent widths from 100 random realizations of the Ne I atomic data. The “observed” equivalent widths corresponded to $\Delta_{\text{MC}} = 8.05$ and $\zeta_t = 5$ km s$^{-1}$.
stars, no Ne I line is detected, and one star falls off the hot end of the computational grid. The error bars on the abundances represent estimated total uncertainties including errors in the fundamental parameters; the specific case of HD 886, representative of the lower end of the $T_{\text{eff}}$ range, is summarized in Table 8. There is a tendency for the derived abundances to be slightly higher than solar for lower $T_{\text{eff}}$, but this trend is perhaps not highly significant given the errors. In addition, there is considerable uncertainty in the solar neon abundance because of the lack of photospheric and meteoritic estimates, as noted in § 1. The large scatter at higher $T_{\text{eff}}$ may result from difficulties in obtaining accurate equivalent widths for extremely weak lines (EW < 10 mA); the observed equivalent widths are shown in the bottom panel of Figure 7.

Also shown in this figure is the neon abundance derived for $\pi$ Ceti from the equivalent width of $\lambda$6402 (54 mA) and stellar parameters of Adelman (1984). The abundance, $8.33 \pm 0.25$ dex, is consistent with the solar abundance within the mutual error bounds. The makeup of the total uncertainty is also given in Table 8. Equivalent widths for four lines of Ne I for 21 Aql are also available from Adelman (1984), but they give extremely discordant abundances ($\lambda$6402, 7.35 ± 0.16; $\lambda$6334, 7.91 ± 0.16; $\lambda$6506, 7.85 ± 0.16; and $\lambda$6598, 8.28 ± 0.16) ranging over nearly a factor of 10, far in excess of the expected errors in each of the individual lines. This is likely due to large uncertainties in the small equivalent widths ranging from 14 to 18 mA. For this reason, 21 Aql is not plotted in Figure 7.

As can be seen from Figure 7, if one considers only objects with $T_{\text{eff}} \lesssim 25,000$ K, the neon abundance obtained is roughly 8.3 dex or log (Ne/H) = −3.7, about 60% higher than the current accepted solar neon abundance (Grevesse & Anders 1992). Neon abundances for early-type B and

---

**TABLE 8**

**Total Uncertainties in Ne I Abundances**

| Parameter      | Uncertainty ($\pi$ Ceti) | Uncertainty (HD 886) |
|----------------|--------------------------|----------------------|
|                | (\lambda 6402)          | (\lambda 6402)      | (\lambda 6506)          | (\lambda 6506)      |
| EW<sub>theory</sub> (mA) | ± 10.0                   | ± 4.5               | ± 1000                  | ± 10.0               |
| $T_{\text{eff}}$ (K)        | ± 250                    | ± 0.25              | ± 0.25                  | ± 0.25               |
| log $g$            | ± 0.25                   | ± 0.16              | ± 0.10                  | ± 0.10               |
| $\zeta_t$ (km s<sup>−1</sup>) | ± 2.0                    | ± 0.08              | ± 0.25                  | ± 0.03               |
| EW<sub>obs</sub> (mA)      | ± 5.0                    | ± 0.10              | ± 0.12                  | ± 0.12               |
| Total              | ± 0.27                   | ± 0.27              | ± 0.19                  | ± 0.19               |

**Note.**—Fundamental stellar parameters adopted for $\pi$ Ceti are $T_{\text{eff}} = 13,150$ K, log $g = 3.65$, and $\zeta_t = 0$ km s<sup>−1</sup>. Those for HD 886 are $T_{\text{eff}} = 22,670$ K, log $g = 4.02$, and $\zeta_t = 0$ km s<sup>−1</sup>.
late-type O stars in open clusters are available from Kilian-Montenbruck et al. (1994) based on the LTE analysis of Ne \( ^{II} \) lines. The current derived value of \( \log (\text{Ne}/H) = -3.7 \) falls near the middle of the observed range for the nearest open clusters, those within \( 7 \) kpc. However, the Ne \( ^{II} \) line strengths need to be the subject of a non-LTE calculation before this fact can be accepted as proof of the consistency of the non-LTE calculation. In addition, it would be reassuring to base the current neon abundances on more than a single line.

4. CONCLUSIONS

A new grid of non-LTE equivalent widths for Ne \( ^{I} \) has been presented for stellar parameters covering the entire range of B stars. These equivalent widths have been explicitly demonstrated to have converged with respect to further increases in model atom complexity. Uncertainties in the predicted line strengths are estimated by Monte Carlo simulation, in which a series of atomic models are randomly realized from the estimated uncertainty distributions of the default atomic data. It is found that for realistic observing programs, the limiting accuracy to neon abundance determinations from lines of Ne \( ^{I} \) due to uncertainties in the atomic data is \( \sim \pm 0.1 \) dex.

New observations of multiple transitions of neon over the entire range of B stars are required. Such a data set, when combined with the presented equivalent width grid, will allow a new estimate of the neon abundance in the local Galactic environment, thus improving current estimates of the solar (photospheric) neon abundance. New observations will also allow us to test the hypothesis that neon over-abundance traces weak stellar winds in late- and mid-B stars and to potentially detect these winds.

The complete grid of equivalent widths for Ne \( ^{I} \) for the range of stellar parameters in Table 1 is available from the author upon request.

It is a pleasure to thank J. D. Landstreet and J. M. Marlborough for helpful discussions and for supporting this research through their NSERC grants. I would also like to thank M. J. Seaton for advice on the Ne \( ^{I} \) atomic data and for letting me use his Ne \( ^{I} \) atomic data prior to publication. Thanks go to Colleen Schinkel for performing the thermal averaging of the available Ne \( ^{I} \) collision strengths.

REFERENCES

Achmad, L., de Jager, C., & Nieuwenhuijzen, H. 1991, A&A, 250, 445
Adelman, S. A. 1984, MNRAS, 206, 637
Auer, L. H., & Mihalas, D. 1973a, ApJS, 25, 433
Auer, L. H., & Mihalas, D. 1973b, ApJ, 184, 151
Bertin, P., Lamers, H. J. G. L. M., Vidal-Madjar, A., Ferlet, R., & Lallement, R. 1995, A&A, 202, 389
Carlsson, M. 1986, A Program for Solving Multilevel Non-LTE Radiative Transfer Problems in Moving Atmospheres (Uppsala Obs. Rep. 33)
Carlsson, M. 1986, A Program for Solving Multilevel Non-LTE Radiative Transfer Problems in Moving Atmospheres (Uppsala Obs. Rep. 33)
—. 1992, in ASP Conf. Ser. 26, Cool Stars, Stellar Systems, and the Sun, ed. M. S. Giampapa & A. Bookbinder (San Francisco: ASP), 499
Cunto, W., Mendoza, C., Ochsenbein, F., & Zeippen, C. J. 1993, A&A, 275, L5
Dimitrijević, M. S., & Konjević, N. 1986, A&A, 163, 297
Gies, D. R., & Lambert, D. L. 1992, ApJ, 387, 673
Grevesse, N., & Anders, E. 1991, in Solar Interior and Atmosphere, ed. A. N. Cox, W. C. Livingston, & M. S. Matthews (Tucson: Univ. Arizona Press), 1227
Grevesse, N., & Sauval, A. J. 1998, in The Solar Neighborhood, ed. H. V. Menzel, & C. L. Aller (Tucson: Univ. Arizona Press), 63
Hibbert, A., & Scott, M. P. 1994, J. Phys. B, 27, 1315
Kilian-Montenbruck, T., Gehren, T., & Nissen, P. E. 1994, A&A, 291, 757
Kurucz, R. L. 1992, in IAU Symp. 149, The Stellar Populations of Galaxies, ed. B. Barbuy & A. Renzini (Dordrecht: Kluwer), 225
Landstreet, J. D., Dolez, N., & Vauclair, S. 1998, A&A, 333, 977
Maciel, W. J., & Köppen, J. 1994, A&A, 282, 436
Meyer, J. P. 1989, in Cosmic Abundances of Matter, ed. C. J. Waddington (New York: AIP), 245
Mihalas, D. 1978, Stellar Atmospheres (New York: Freeman)
Moore, C. E. 1994, Atomic Energy Levels, Vol. 1 (NBS Circ. 467; Washington, DC: GPO)
Oertel, G. K., & Shomo, L. P. 1968, ApJS, 16, 175
Phillips, M. H., Anderson, L., & Lin, C. C. 1985, Phys. Rev. A, 32, 2117
Pradhan, A. K., & Gallagher, J. W. 1992, At. Data Nucl. Data Tables, 52, 227
Sampson, D. H., & Zhang, H. L. 1992, Phys. Rev. A, 45, 1556
Sawey, P. M. J., Berrington, K. A., Burke, P. G., & Kingston, A. E. 1990, J. Phys. B., 23, 4321
Seaton, M. J. 1998a, J. Phys. B, 31, 5315
———. 1999b, MNRAS, 300, L1
———. 1997, J. Phys. B, 20, 6431
———. 1988, J. Phys. B, 21, 3033
———. 1986, Proc. Phys. Soc. London, 79, 1105
Sigut, T. A. A. 1996, ApJ, 473, 452
Sigut, T. A. A., & Lester, J. B. 1996, ApJ, 473, 452
Simpson, J. P., Colgan, S. W., Rubin, R. H., Erickson, E. F., & Haas, M. R. 1994, ApJ, 444, 721
Sobotka, L. 1962, Proc. Phys. Soc. London, 79, 1105
Sobotka, L. 1963, Proc. Phys. Soc. London, 79, 1105
Sobelman, I. I. 1981, Atomic Spectra and Radiative Transitions (Berlin: Springer)
Taylor, K. T., Clark, C. W., & Fon, W. C. 1985, J. Phys. B, 18, 2967
Van Regemorter, H. 1960, ApJ, 121, 213
Zeman, V., & Bartschat, K. 1997, J. Phys. B, 30, 4609 (ZB97)