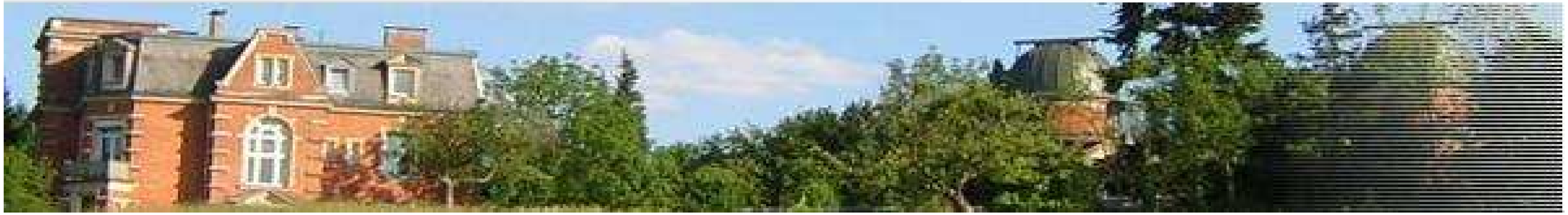
Dr. Remeis-Sternwarte Bamberg
Astronomical Institute of the
University of Erlangen-Nuremberg



Model Atom Construction

General Considerations
Literature on Model Atoms

N. Przybilla

Requirements for accurate analyses

- local temperature & particle densities need to be known

  → atmospheric structure

- radiation field realistic

  → $S_\nu \neq B_\nu(T)$

- all relevant processes taken into account for SE

- high-quality atomic data available

  → ab-initio calculations

model atoms

→ any weakness affects overall accuracy

Definition

Model atom: A collection of atomic data
- energy levels & cross-sections -
that allows the interaction of a real atom/ion with
radiation and colliding particles in a plasma
to be modelled.

Processes:

- radiative bound-bound	RBB	non-local
- radiative bound-free	RBF	
- collisional bound-bound	CBB	local
- collisional bound-free	CBF	

+ charge exchange, dielectronic recombination, ...

Uncertainty in one quantity cannot be compensated by accuracy in other quantity.

Completness of model atom – how many levels to include?

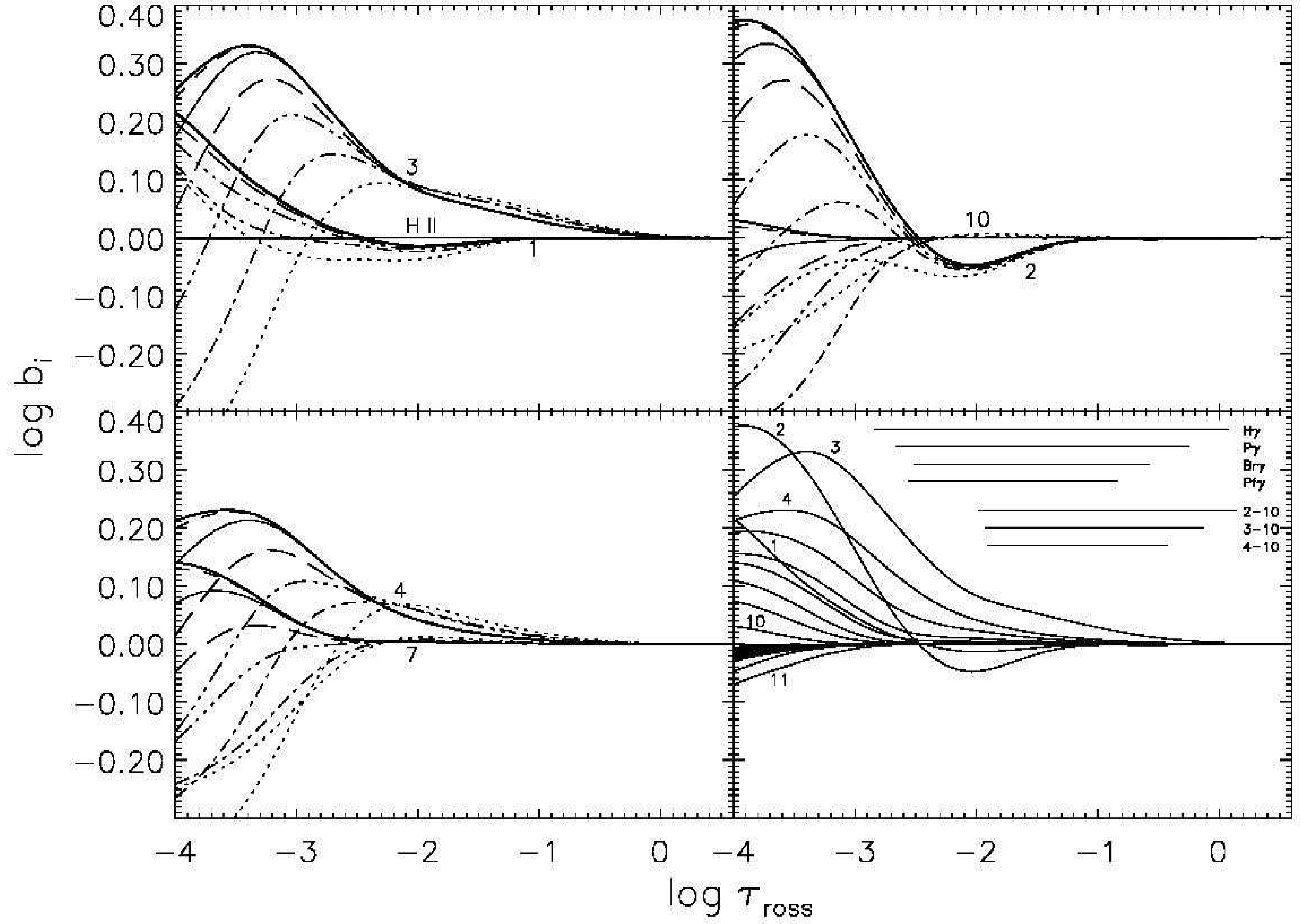
- as many as necessary

- realisation:
  - fine-structure states
  - terms
  - superlevels

- convergence criteria:
  - for increasing number of levels:
    b_i and related quantities approach limiting value
  - b_i of high-excitation levels approach
    b of ground state of next ionization stage

Completness of model atom

Przybilla & Butler 2004, ApJ, 609, 1181



- H: convergence behaviour b_i for 10, 15, 20, 25, 30, 40, 50-level atom

Completness of model atom

- convergence of line source function, equivalent width

Sigut 1996, ApJ, 473, 452

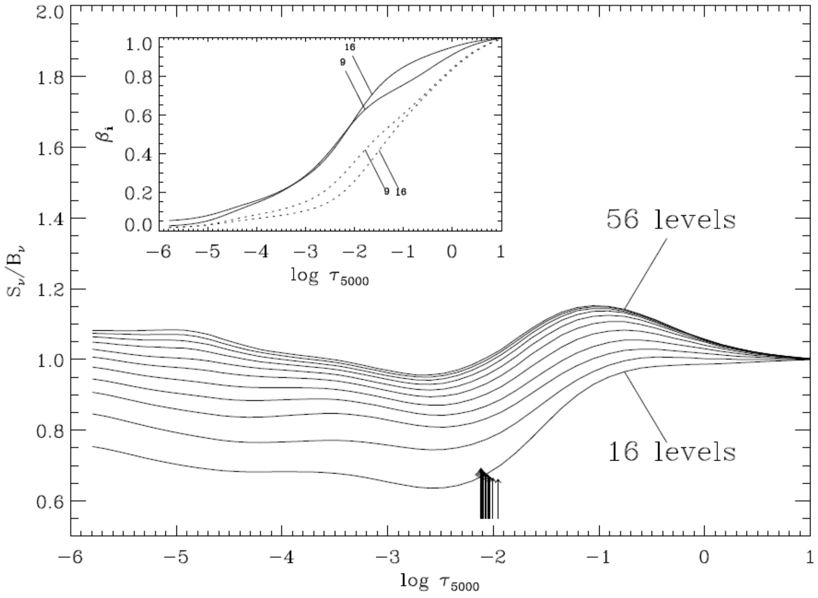


FIG. 3.—The line center monochromatic source function for 4267 Å at $T_{\rm eff} = 25{,}000$ K, log $(g) = 4.0$, $\zeta_t = 5$ km s^{-1}. Shown are the predictions of increasing complex model atoms corresponding to the diamonds of Fig. 4. Arrows in the main figure indicate the depth of formation of the emergent line radiation at line center. The insert shows the departure coefficients of the upper and lower multiplet levels as predicted by 16 (*dotted curve*) and 56 (*solid curve*) C II model atoms. The departure coefficients are defined as $\beta_i = n_i/n_i^*$ where an asterisk denotes the LTE population.

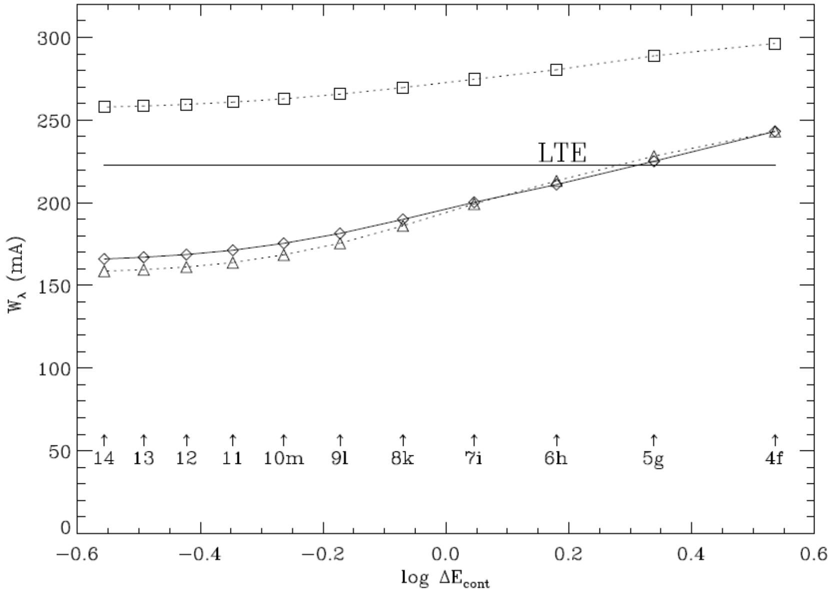


FIG. 4.—The influence of model atom complexity on the equivalent width of 4267 Å at $T_{\rm eff} = 25{,}000$ K, log $(g) = 4.0$, $\zeta_t = 5$ km s^{-1}. $\Delta E_{\rm cont}$ is the gap in electron volts between the last included non-LTE level and the C III continuum. Shown are the predictions of models atoms complete in energy levels and radiative transitions to the indicated levels (*open diamonds*), model atoms complete in energy levels but retaining only the 35 radiative transitions of the 16 level model atom (*open triangles*), and model atoms complete in energy levels and radiative transition but with photoionization rates from levels 6, 7, 9, and 16 set in detailed balance (*open squares*).

Transitions – which to include, using which data?

- all relevant

- measurements:
  - energy levels
  - oscillator strengths
  - photoionization cross-sections from ground (metastable) states
  - collisional excitation/ionization cross-sections from ground (metastable) states

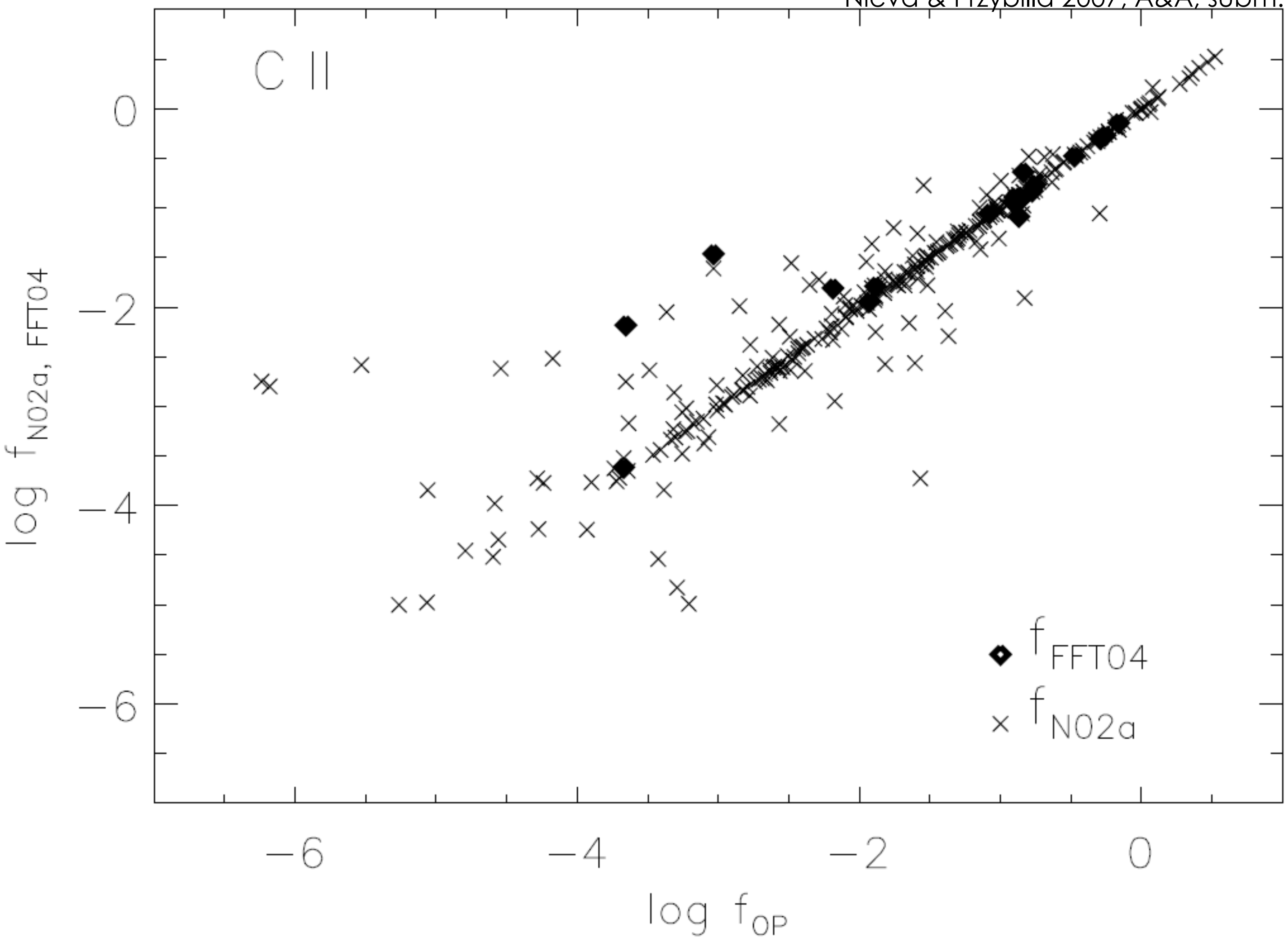
- ab-initio data:
  - oscillator strengths, photoionization cross-sections
  - (effective) collision strengths (electron collisions)

- approximations:
  - THE REST (including collisions with neutral H)

RBB's

- comparison of different results from ab-initio calculations

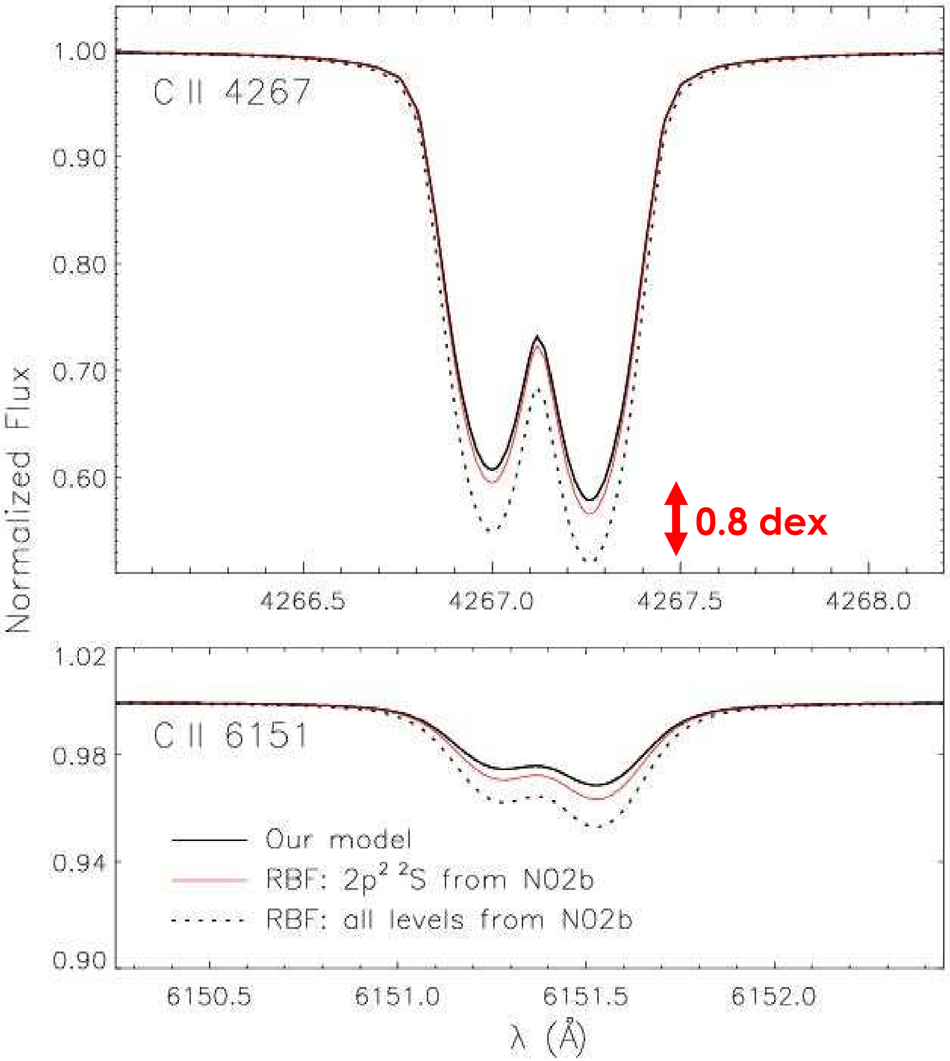
Nieva & Przybilla 2007, A&A, subm.

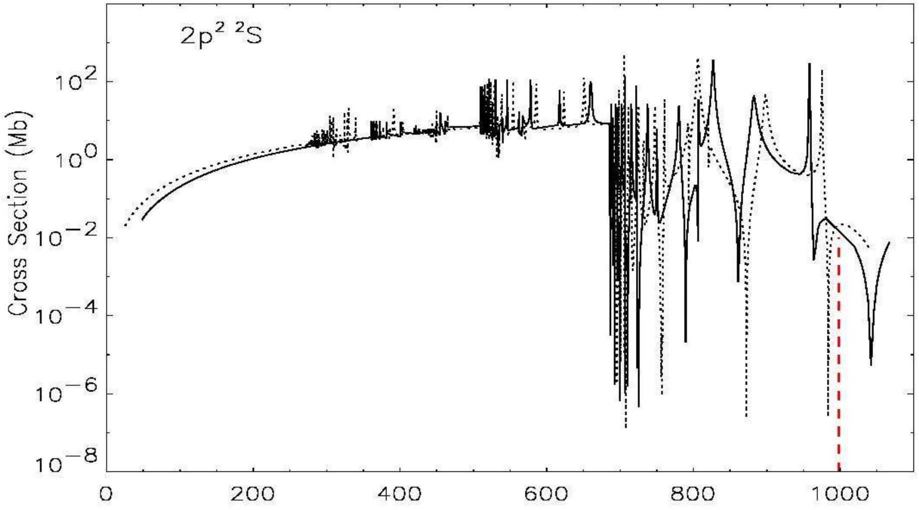


- your responsibility which data to trust: always check

RBF's

Nieva & Przybilla 2007, A&A, subm.



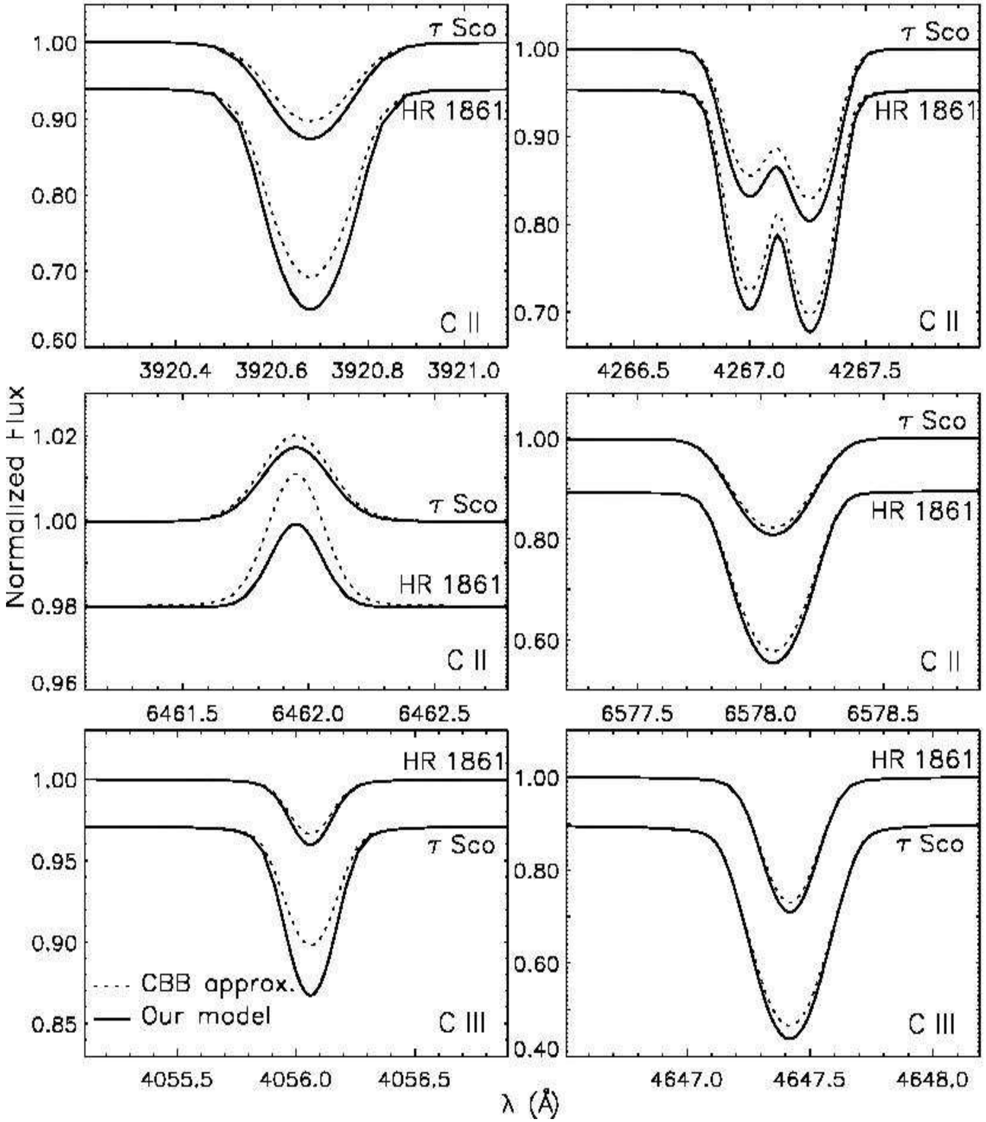


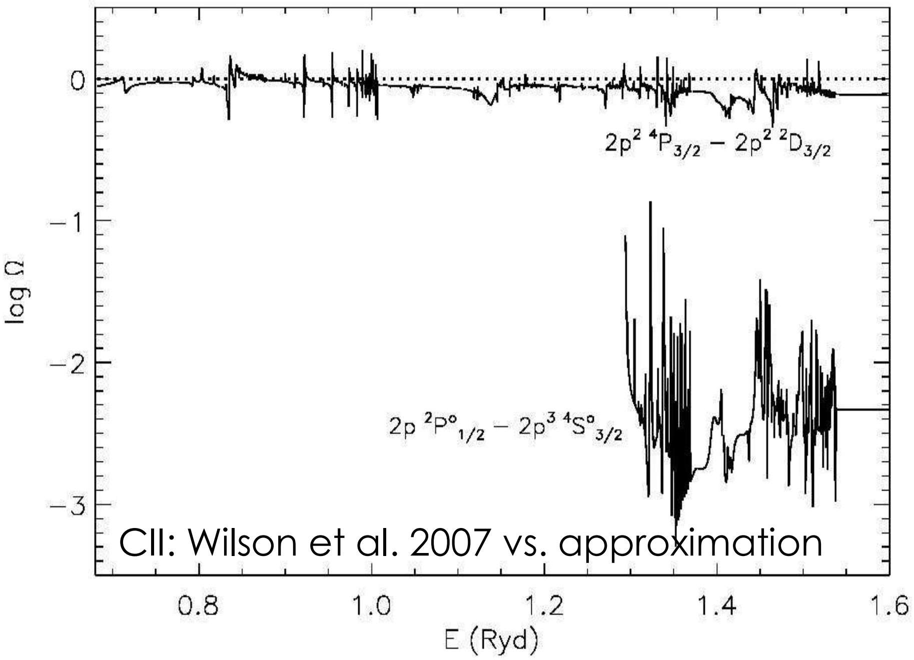
- efficient drivers out of LTE, impact well-populated low-lying levels
- ionization thresholds important
- resonance structure vs. averages

→ check your data

CBB's

Nieva & Przybilla 2007, A&A, subm.



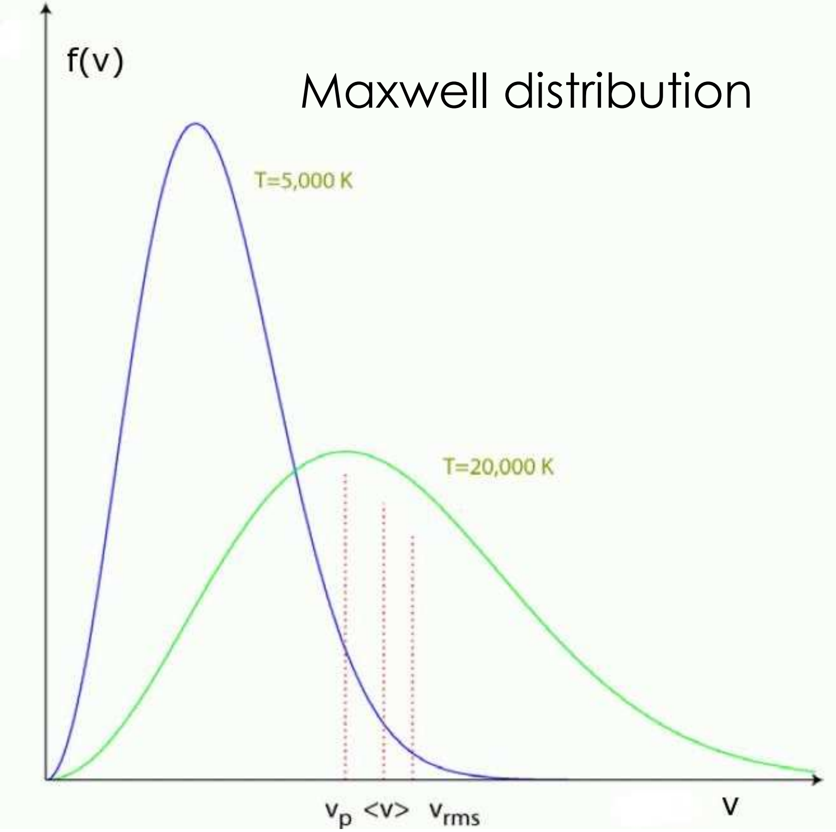


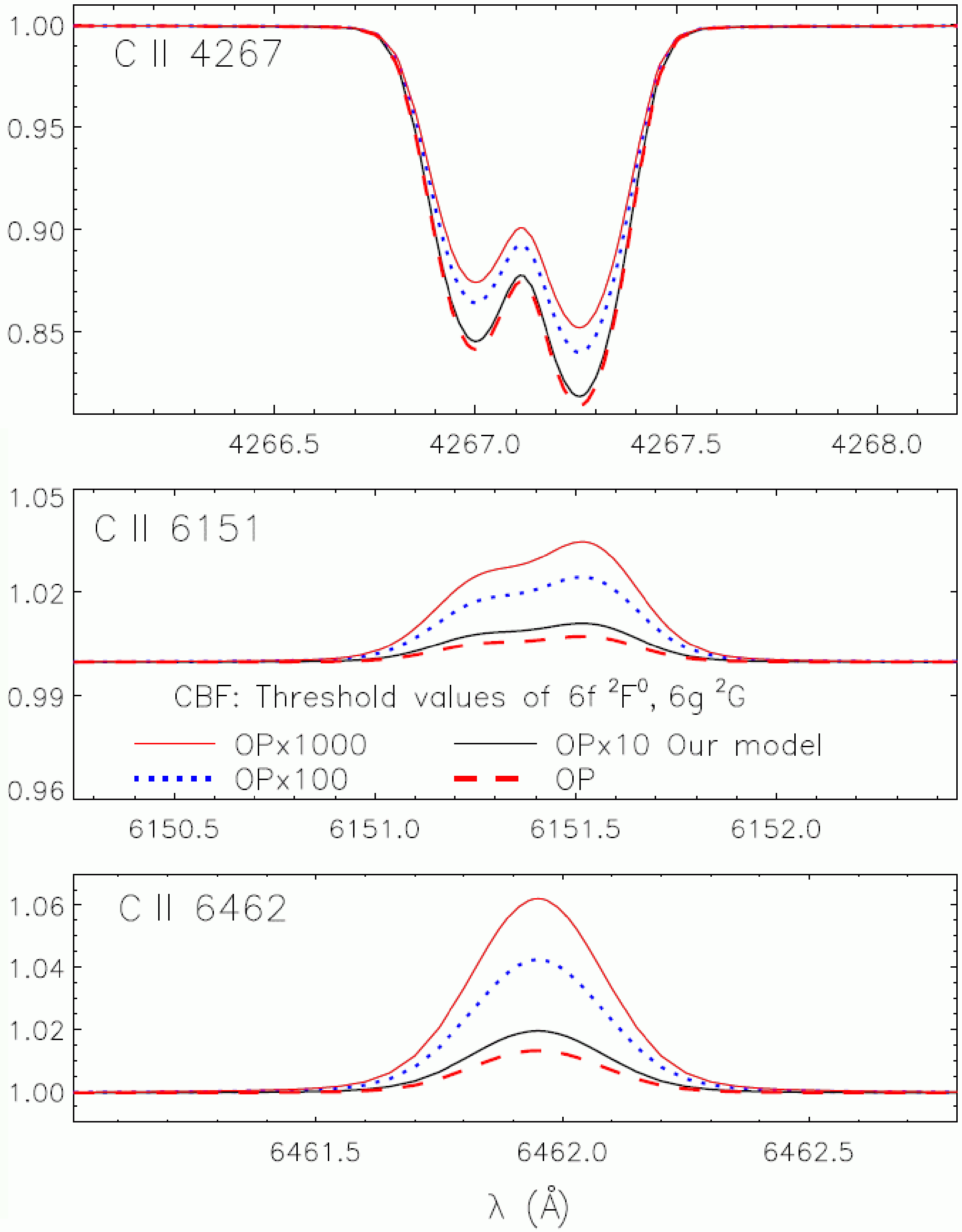
CII: Wilson et al. 2007 vs. approximation

- fine-tuning of b-factors
- large impact on lines possible
- high-quality data becoming available in larger quantities only recently

CBF's

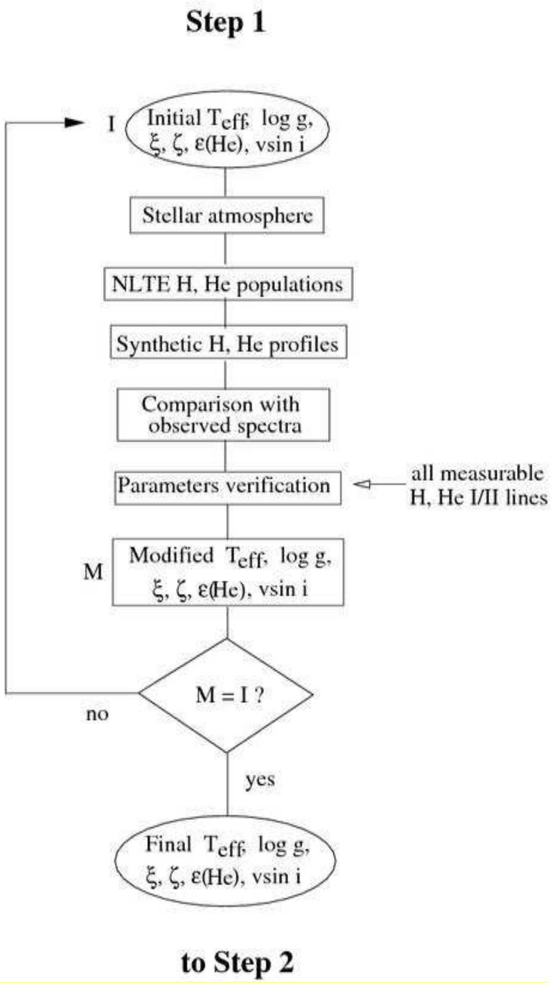
- relatively unimportant for well-populated low-lying levels
- highly important for collisional coupling to higher ionization stage

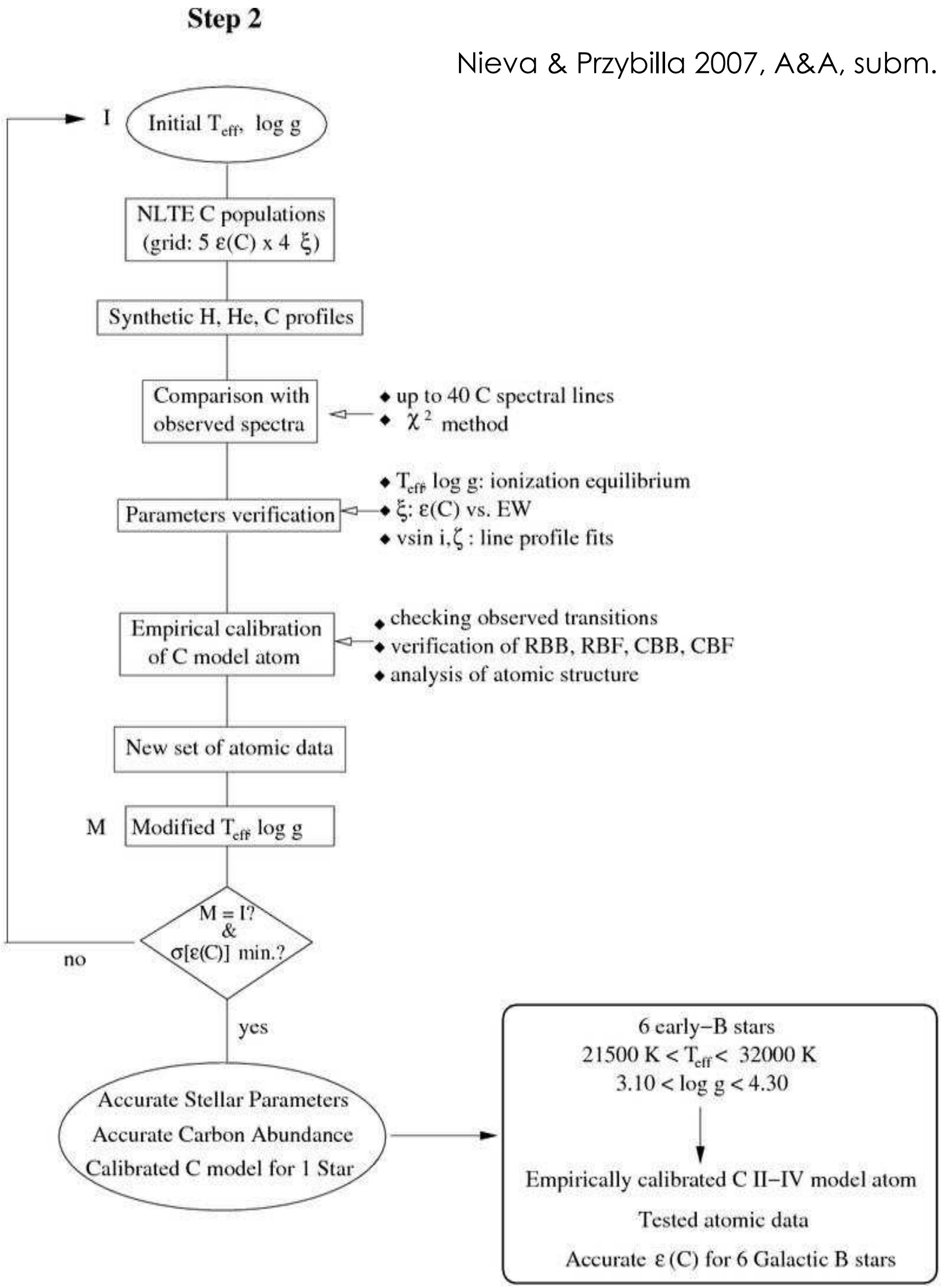



Nieva & Przybilla 2007, A&A, subm.

Model atom construction: a comprehensive approach

Nieva & Przybilla 2007, A&A, subm.

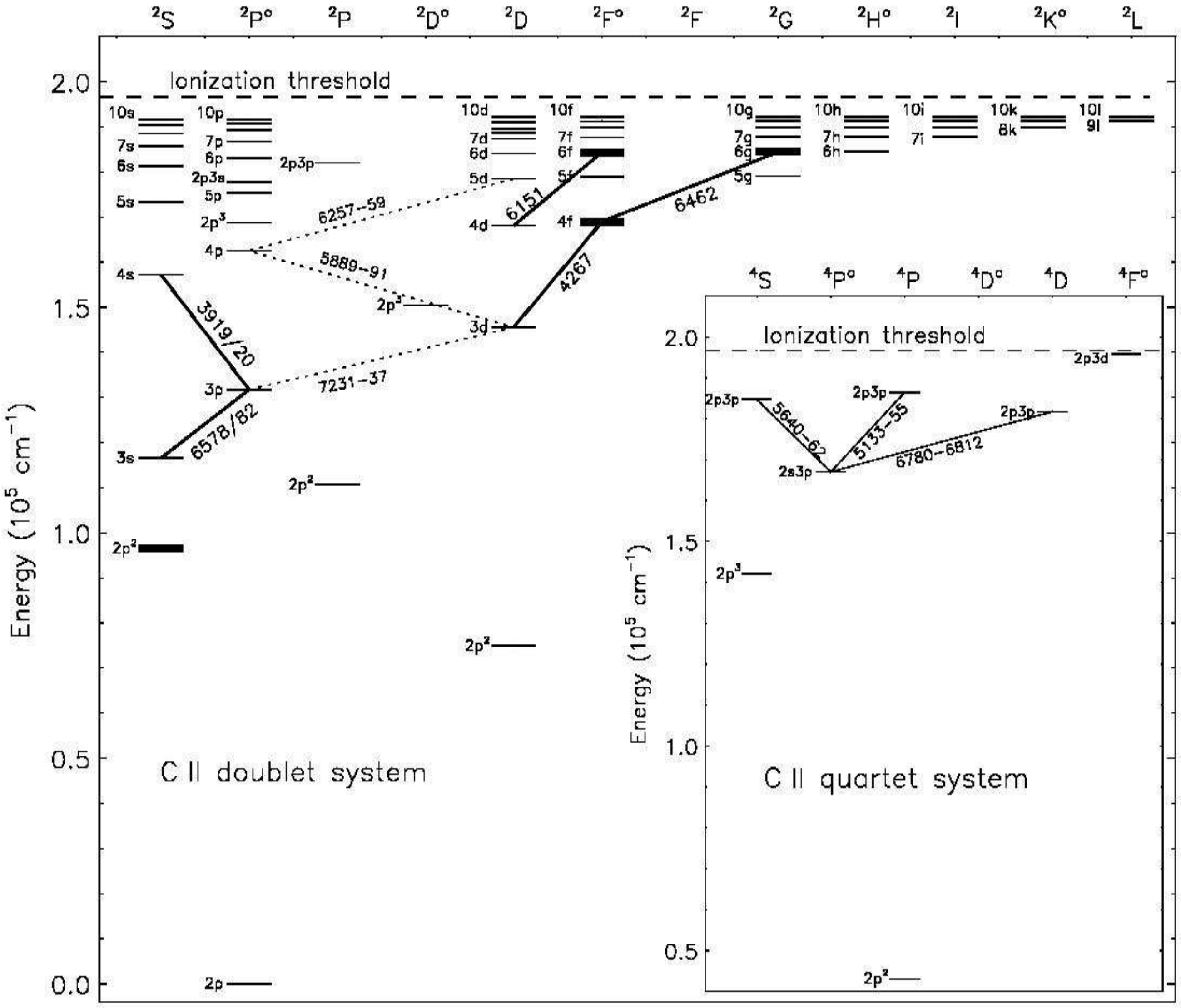




simultaneous determination of atmospheric parameters & calibration of model atom

Atomic structure

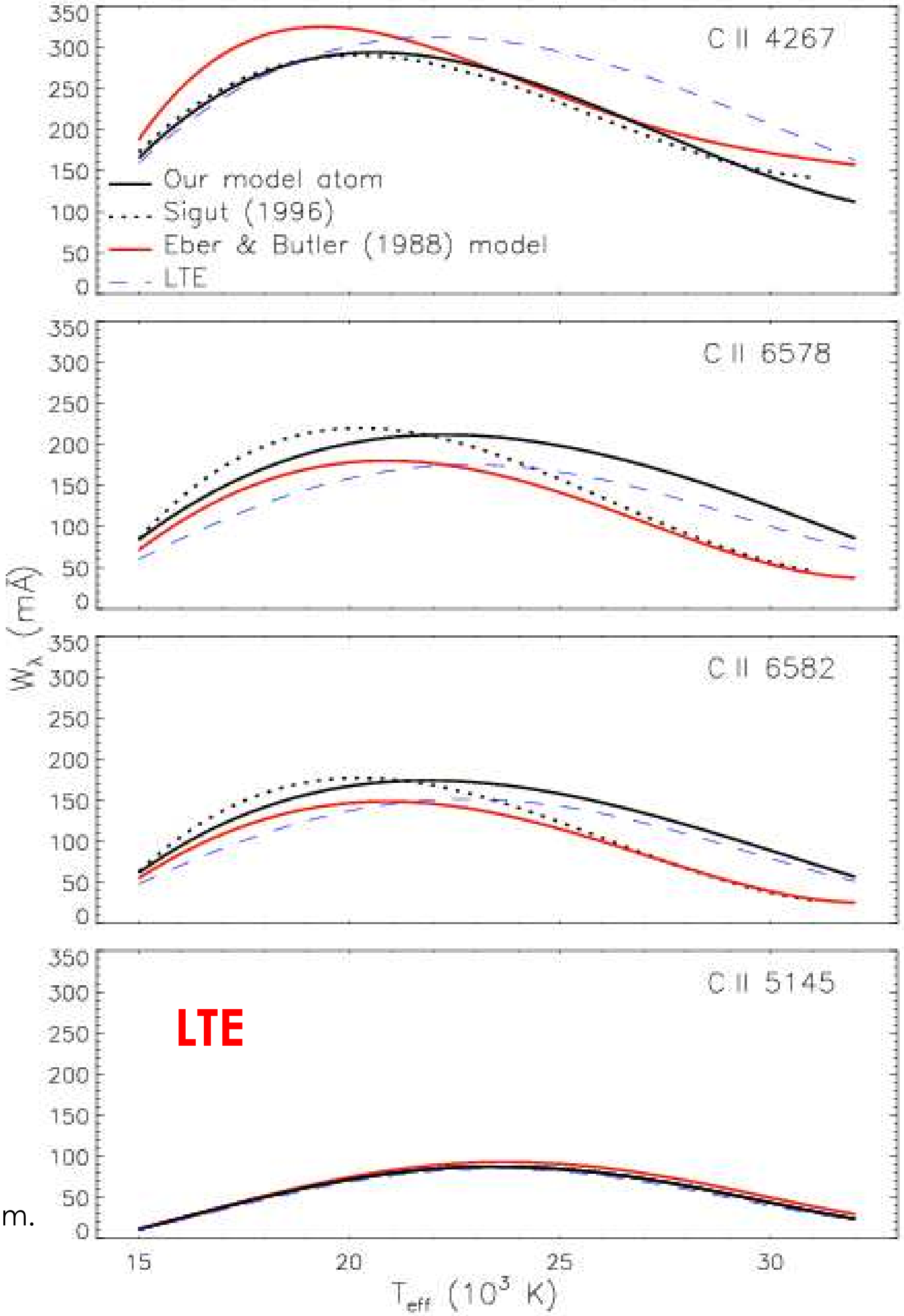
Nieva & Przybilla 2007, A&A, subm.



- Grotrian diagrams help to identify important channels

Systematic trends

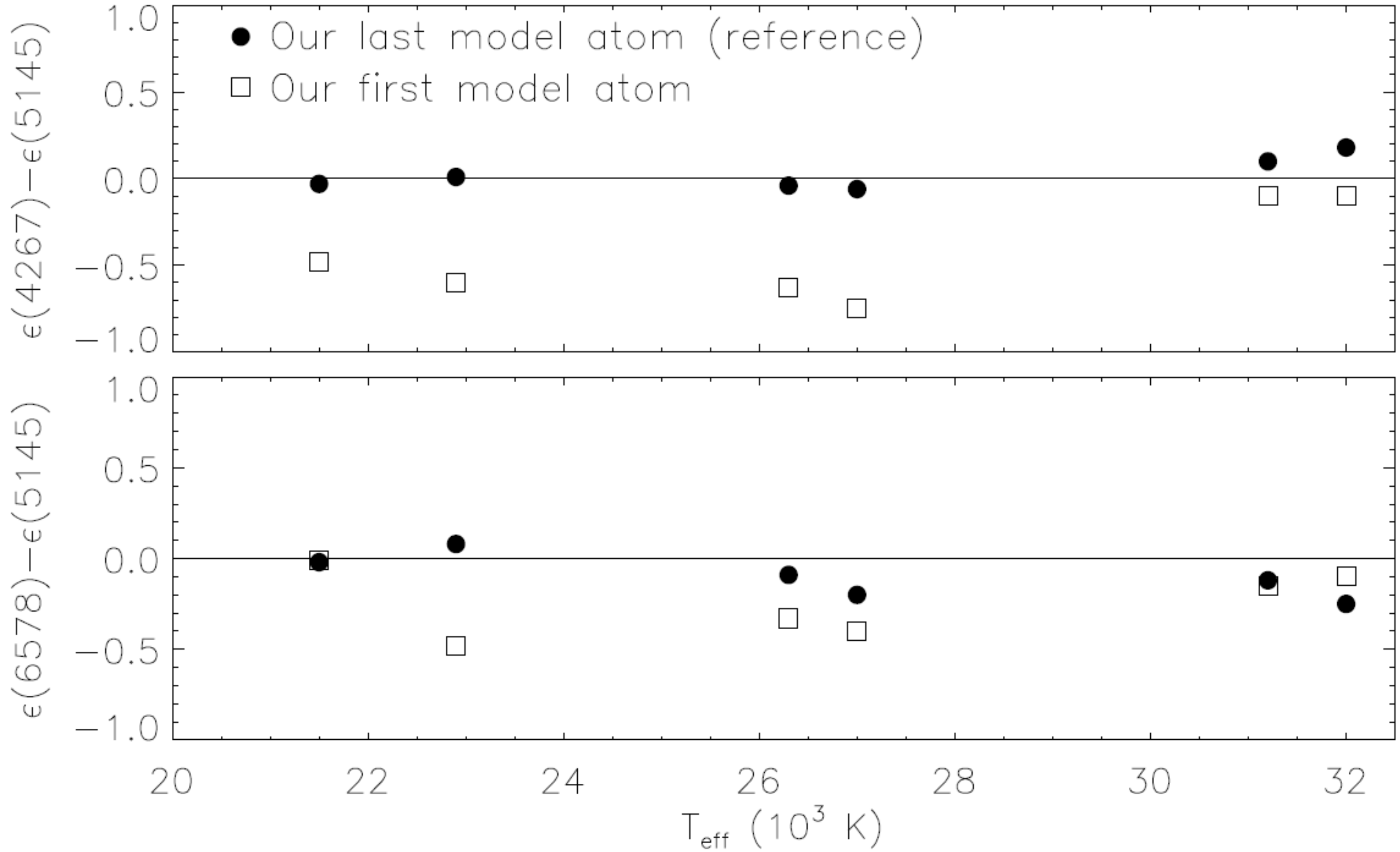
- some lines essentially in LTE
  → independent of (any reasonable) choice of atomic data
- highly useful for fixing abundance as standard for calibration of atomic data for NLTE lines
- base calibration on observation spreading large range in atmospheric parameters: **atomic data independent of environment**



Nieva & Przybilla 2007, A&A, subm.

Optimisation of model atoms by empirical calibration

Nieva & Przybilla 2007, A&A, subm.



- via minimisation of abundance spread, i.e. random error from individual lines ➞ at best: ~10-20% uncertainty (1σ) in absolute abundance

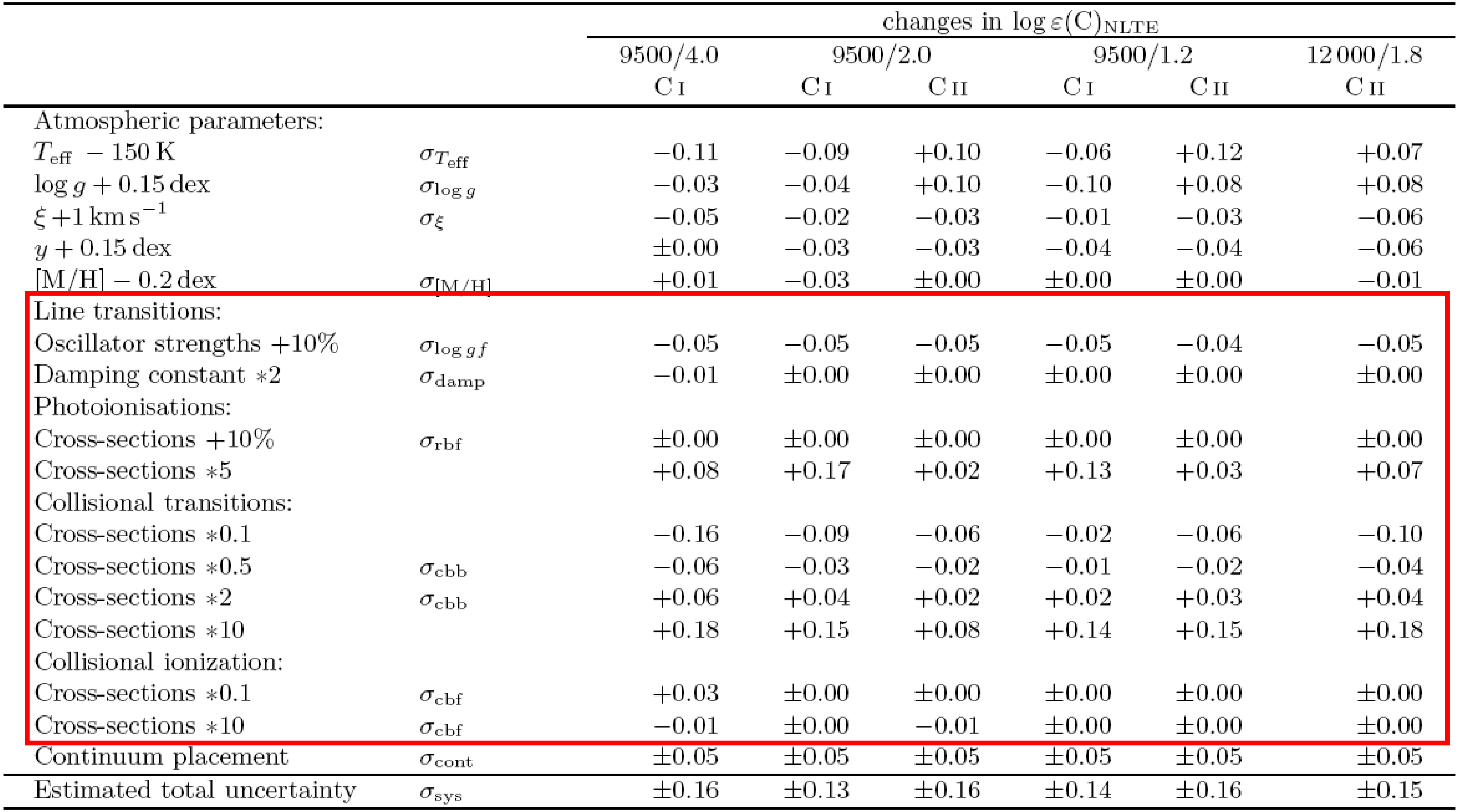
Robustness of model atoms: systematic uncertainties

- contribution of atomic data uncertainties
  to overall uncertainty of abundance determination

- time consuming: many test calculations with varied
  atomic input data required

Determination of systematic uncertainties

Przybilla et al. 2001, A&A, 379, 936

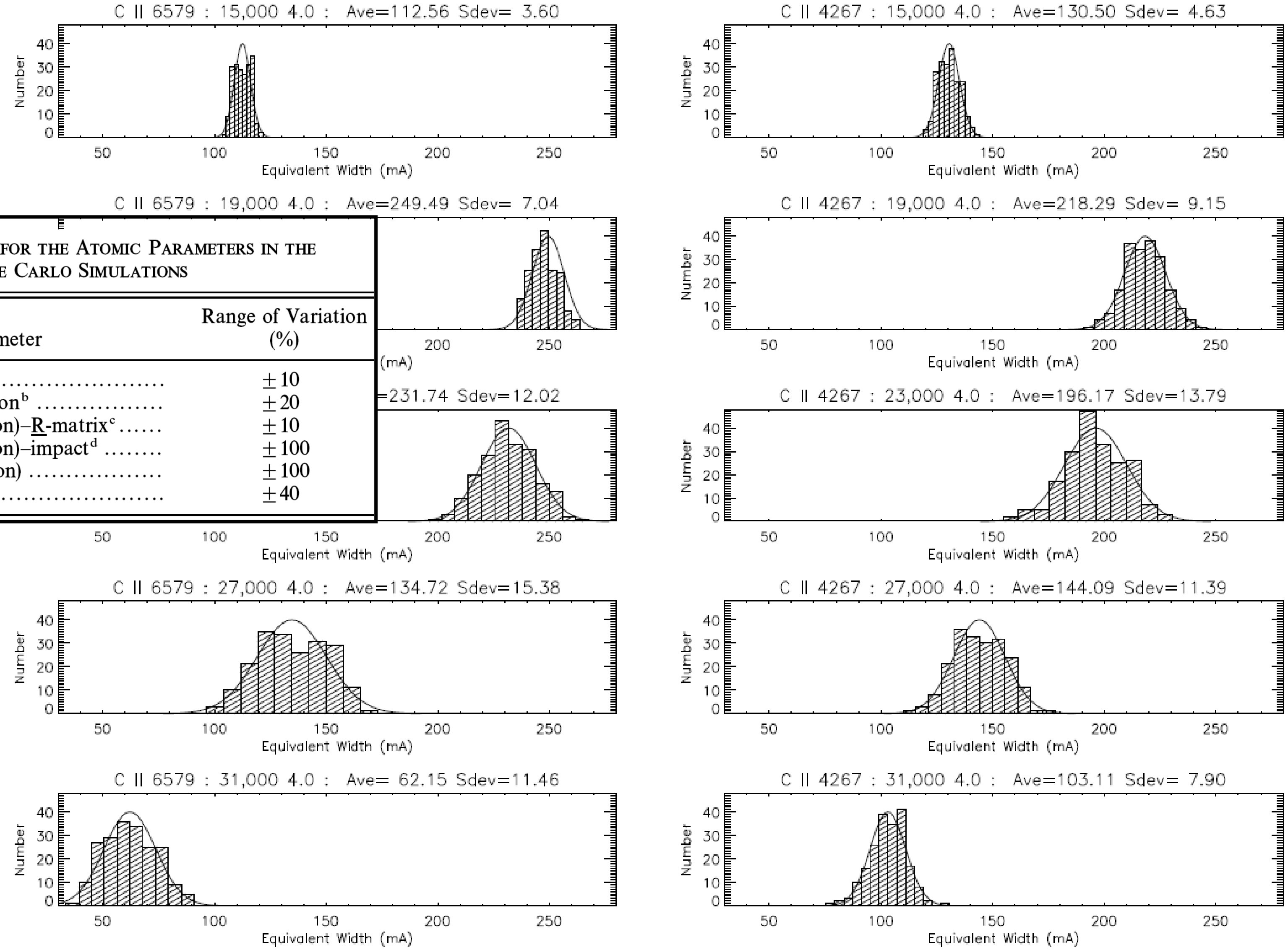


		changes in $\log \varepsilon(\mathrm{C})_{\mathrm{NLTE}}$					
		9500/4.0	9500/2.0		9500/1.2		12 000/1.8
		C I	C I	C II	C I	C II	C II
Atmospheric parameters:							
T_{eff} $-$ 150 K	$\sigma_{T_{\mathrm{eff}}}$	−0.11	−0.09	+0.10	−0.06	+0.12	+0.07
$\log g + 0.15$ dex	$\sigma_{\log g}$	−0.03	−0.04	+0.10	−0.10	+0.08	+0.08
ξ +1 km s^{-1}	σ_{ξ}	−0.05	−0.02	−0.03	−0.01	−0.03	−0.06
$y + 0.15$ dex		±0.00	−0.03	−0.03	−0.04	−0.04	−0.06
[M/H] − 0.2 dex	$\sigma_{[\mathrm{M/H}]}$	+0.01	−0.03	±0.00	±0.00	±0.00	−0.01
Line transitions:							
Oscillator strengths +10%	$\sigma_{\log gf}$	−0.05	−0.05	−0.05	−0.05	−0.04	−0.05
Damping constant *2	σ_{damp}	−0.01	±0.00	±0.00	±0.00	±0.00	±0.00
Photoionisations:							
Cross-sections +10%	σ_{rbf}	±0.00	±0.00	±0.00	±0.00	±0.00	±0.00
Cross-sections *5		+0.08	+0.17	+0.02	+0.13	+0.03	+0.07
Collisional transitions:							
Cross-sections *0.1		−0.16	−0.09	−0.06	−0.02	−0.06	−0.10
Cross-sections *0.5	σ_{cbb}	−0.06	−0.03	−0.02	−0.01	−0.02	−0.04
Cross-sections *2	σ_{cbb}	+0.06	+0.04	+0.02	+0.02	+0.03	+0.04
Cross-sections *10		+0.18	+0.15	+0.08	+0.14	+0.15	+0.18
Collisional ionization:							
Cross-sections *0.1	σ_{cbf}	+0.03	±0.00	±0.00	±0.00	±0.00	±0.00
Cross-sections *10	σ_{cbf}	−0.01	±0.00	−0.01	±0.00	±0.00	±0.00
Continuum placement	σ_{cont}	±0.05	±0.05	±0.05	±0.05	±0.05	±0.05
Estimated total uncertainty	σ_{sys}	±0.16	±0.13	±0.16	±0.14	±0.16	±0.15

P.S.: ~1 month of CPU time for this ...

Uncertainties: Monte-Carlo Simulations

Sigut 1996, ApJ, 473, 452



Variation Adopted for the Atomic Parameters in the Monte Carlo Simulations

Atomic Parameter	Range of Variation (%)
f-value[a]	±10
Photoionization cross section[b]	±20
Collision strength (excitation)–R-matrix[c]	±10
Collision strength (excitation)–impact[d]	±100
Collision strength (ionization)	±100
Stark width[e]	±40

FIG. 9.—The results of the Monte-MULTI simulation. The histograms have bin widths of one-half standard deviation. All simulations had 200 runs. All of the distributions are well fitted by a Gaussian (based on a χ^2 test), shown as the solid lines, except for 6579 Å at $T_{\rm eff}$ = 15,000 K.

Conclusions

- construction of model atoms: complex, time-consuming task
- use of ‘most recent‘ atomic data not sufficient:
  required is most accurate
  → any weakness impacts overall accuracy
- calibration vs. observation:
  the more empirical constraints the better
- calibration over wide range of plasma parameters:
  atomic data independent of environment

Appendix: Literature on NLTE model atoms

H:
Barklem, P.S. 2007, A&A, 466, 327
Carlsson, M., & Rutten, R.J. 1992, A&A, 259, L53
Husfeld, D., Butler, K., Heber, U., & Drilling, J.S. 1989, A&A, 222, 150
Przybilla, N., & Butler, K. 2004, ApJ, 609, 1181

He:
Husfeld, D., Butler, K., Heber, U., & Drilling, J.S. 1989, A&A, 222, 150 (He I/II)
Leone, F., Lanzafame, A.C., & Pasquini, L. 1995, A&A, 293, 457 (He I)
Przybilla, N. 2005, A&A, 443, 293 (He I)
Sakhibullin, N. A., & Schabert, W. J. 1990, Soviet. Astr. Letters, 16, 231 (He I)
Takeda, Y. 1994, PASJ, 46, 181 (He I)

Li I:
Barklem, P.S., Belyaev, A.K., Asplund, M. 2003, A&A, 409, L1
Carlsson, M., Rutten, R.J., Bruls, J.H.M.J., & Shchukina, N.G. 1994, A&A, 288, 860
Mashonkina, L.I., Shavrina, A.V., Khalack, V., et al. 2002, A. Rep., 46, 27
Shi, J.R., Gehren, T., Zhang, H.W., Zeng, J.L., & Zhao, G. 2007, A&A, 465, 587
Steenbock, W., & Holweger, H. 1984, A&A, 130, 319
Takeda, Y., & Kawanomoto, S. 2005, PASJ, 57, 45

Be:
Garcia Lopez, R.J., Severino, G., & Gomez, M.T. 1995, A&A, 297, 787 (Be I)

B:
Kiselman, D. 1994, A&A, 286, 169 (B I)

C:
Eber, F., Butler, K. 1988, A&A, 202, 153 (C II)
Fabbian, D., Asplund, M., Carlsson, M., Kiselman, D. 2006, A&A, 458, 899 (C I)
Husfeld, D., Butler, K., Heber, U., & Drilling, J.S. 1989, A&A, 222, 150 (C IV)
Lennon, D.J. 1983, MNRAS, 205, 829 (C II)
Nieva, M.F., & Przybilla, N. 2006, ApJ, 639, L39 (C II)
Nieva, M.F., & Przybilla, N. 2007, A&A, submitted (C II-IV)
Przybilla, N., Butler, K., Kudritzki, R.P. 2001, A&A, 379, 936 (C I/II)
Rentzsch-Holm, I. 1996, A&A, 312, 966 (C I)
Sakhibullin, N.A. 1987, Soviet. Astr., 31, 151 (C II)
Sigut, T.A.A. 1996, ApJ, 473, 452 (C II)
Stürenburg, S., & Holweger, H. 1990, A&A, 237, 125 (C I)
Takeda, Y. 1992, PASJ, 44, 649 (C I)

N:
Becker, S.R., & Butler, K. 1989, A&A, 209, 244 (N II)
Husfeld, D., Butler, K., Heber, U., & Drilling, J.S. 1989, A&A, 222, 150 (N III, N V)
Lemke, M., & Venn, K.A. 1996, A&A, 309, 558 (N I)
Przybilla, N., & Butler, K. 2001, A&A, 379, 955 (N I/II)
Rentzsch-Holm, I. 1996, A&A, 305, 275 (N I)
Takeda, Y. 1992, PASJ, 44, 649 (N I)

O:
Becker, S.R., & Butler, K. 1988, A&A, 201, 232 (O II)
Brown, P.J.F., Dufton, P.L., & Lennon, D.J. 1988, MNRAS, 230, 443 (O II)
Carlsson, M., & Judge, P. G. 1993, ApJ, 402, 344
Kiselman, D. 1991, A&A, 245, L9 (O I)
Mishenina, T.V., Korotin, S.A., Klochkova, V.G., & Panchuk, V.E. 2000, A&A, 353, 978 (O I)
Paunzen, E., Kamp, I., Iliev, I. K., et al. 1999, A&A, 345, 597 (O I)
Przybilla, N., Butler, K., Becker, S.R., Kudritzki, R.P., & Venn, K.A. 2000, A&A, 359, 1085 (O I)
Reetz, J. 1999, Ap&SS, 265, 171 (O I)
Takeda, Y. 1992, PASJ, 44, 309 (O I)

Ne:
Sigut, T.A.A. 1999, ApJ, 519, 303 (Ne I)

Na:
Baumüller, D., Butler, K., Gehren, T. 1998, A&A, 338, 637 (Na I)
Boyarchuk, A.A., Hubeny, I., Kubat, J., Lyubimkov, L.S., & Sakhibullin, N.A. 1988, Astrofizika, 28, 335 (Na I)
Bruls, J.H.M.J., Rutten, R.J., & Shchukina, N.G. 1992, A&A, 265, 237 (Na I)
Mashonkina, L., Sakhibullin, N. A., & Shimanskii, V. V. 1993, A. Rep., 37, 192 (Na I)
Sakhibullin, N.A. 1987, Soviet. Astr., 31, 666 (Na I)
Takeda, Y., & Takada-Hidai, M. 1994, PASJ, 46, 395 (Na I)

Mg:
Abia, C., & Mashonkina, L. 2004, MNRAS, 350, 1127 (Mg II)
Carlsson, M., Rutten, R.J., & Shchukina, N.G. 1992, A&A, 253, 567 (Mg I)
Gigas, D. 1988, A&A, 192, 264 (Mg I/II)
Idiart, T., & Thévenin, F. 2000, ApJ, 541, 207 (Mg I)
Lemke, M., & Holweger, H. 1987, A&A, 173, 375 (Mg I)
Mashonkina, L.I., Shimanskaya, N.N., & Sakhibullin, N.A. 1996, A. Rep., 40, 187 (Mg I)
Przybilla, N., Butler, K., Becker, S.R., & Kudritzki, R.P. 2001, A&A, 369, 1009 (Mg I/II)
Sigut, T.A.A., & Lester, J.B. 1996, ApJ, 461, 972 (Mg II)
Zhao, G., Butler, K., & Gehren, T. 1998, A&A, 333, 219 (Mg I)

Al:
Baumüller, D., & Gehren, T. 1996, A&A, 307, 961 (Al I)
Dufton, P.L., Brown, P.J.F., Lennon, D.J., & Lynas-Gray, A.E. 1986, MNRAS, 222, 713 (Al III)

Si:
Becker, S.R., & Butler, K. 1990, A&A, 235, 326 (Si II-IV)
Lennon, D.J., Brown, P.J.F., Dufton, P.L., & Lynas-Gray, A.E. 1986, MNRAS, 222, 719 (Si II-IV)

S:
Takada-Hidai, M., & Takeda, Y. 1996, PASJ, 48, 739 (S I)
Vrancken, M., Butler, K., Becker, S.R. 1996, A&A, 311, 661 (S II/III)

K:
Bruls, J.H.M.J., Rutten, R.J., & Shchukina, N.G. 1992, A&A, 265, 237 (K I)
Takeda, Yoichi, Kato, K.-I., Watanabe, Y., & Sadakane, K. 1996, PASJ, 48, 511 (K I)
Zhang, H.W., Butler, K., Gehren, T., Shi, J.R., & Zhao, G. 2006, A&A, 453, 723 (K I)

Ca:
Drake, J.J. 1991, MNRAS, 251, 369 (Ca I)
Idiart, T., & Thévenin, F. 2000, ApJ, 541, 207 (Ca I)
Mashonkina, L., Korn, A.J., & Przybilla, N. 2007, A&A, 461, 261 (Ca I/II)
Watanabe, T., & Steenbock, W. 1985, A&A, 149, 21 (Ca I)

Mn:
Sigut, T.A.A. 2001, ApJ, 546, L115 (Mn II)

Fe:
Becker, S.R., & Butler, K. 1992, A&A, 265, 647 (Fe V)
Becker, S.R., & Butler, K. 1995, A&A, 294, 215 (Fe VI)
Becker, S.R., & Butler, K. 1995, A&A, 301, 187 (Fe IV)
Collet, R., Asplund, M., & Thévenin, F. 2005, A&A, 442, 643 (Fe I/II)
Gehren, T., Butler, K., Mashonkina, L., Reetz, J., & Shi, J. 2001, A&A, 366, 981 (Fe I)
Gigas, D. 1986, A&A, 165, 170 (Fe I/II)
Takeda, Y. 1991, A&A, 242, 455 (Fe I/II)
Thévenin, F., & Idiart, T.P. 1999, ApJ, 521, 753 (Fe I/II)

Ni:
Becker, S.R., & Butler, K. 1995, A&A, 300, 453 (Ni IV-VI)

Zn:
Takeda, Y., et al. 2005, PASJ, 57, 751 (Zn I)

Sr:
Belyakova, E.V., & Mashonkina, L.I. 1997, A. Rep., 41, 530 (Sr II)

Ba:
Mashonkina, L., Gehren, T., & Bikmaev, I. 1999, A&A, 343, 519 (Ba II)

Eu:
Mashonkina, L.I. 2000, A. Rep., 44, 558 (Eu II)
Mashonkina, L.I., Ryabtsev, A.N., & Ryabchikova, T.A. 2002,
Ast. Letters, 28, 34 (Eu III)

Nd II/III:
Mashonkina, L., Ryabchikova, T., & Ryabtsev, A. 2005, A&A, 441, 309

Collections of model atoms

Allende Prieto, C., Lambert, D.L., Hubeny, I., & Lanz, T. 2003, ApJS, 147, 363

Li I/II, Be I/II, B I/II, C I/II, N I/II, O I/II, F I/II, Ne II, Na I,
Mg I/II, Al I/II, Si I/II, S I, Ca I/II

Grigsby, J.A., Morrison, N.D., & Anderson, L.S. 1992, ApJS, 78, 205

H, He I/II, C II-IV, N II-IV, O II-IV, Ne I, Mg II

Hubeny, I., & Lanz, T. 2003, ApJS, 146, 417

H, He I/II, C II-IV, N II-V, O II-VI, Ne II-IV, Si III/IV, P IV/V, S III-VI,
Fe III-VI, Ni III-VI

Hubeny, I., & Lanz, T. 2007, ApJS, 169, 83

H, He I/II, C I-IV, N I-V, O I-V, Ne I-IV, Mg II, Al II/III, Si II-IV,
S II-V, Fe II-V