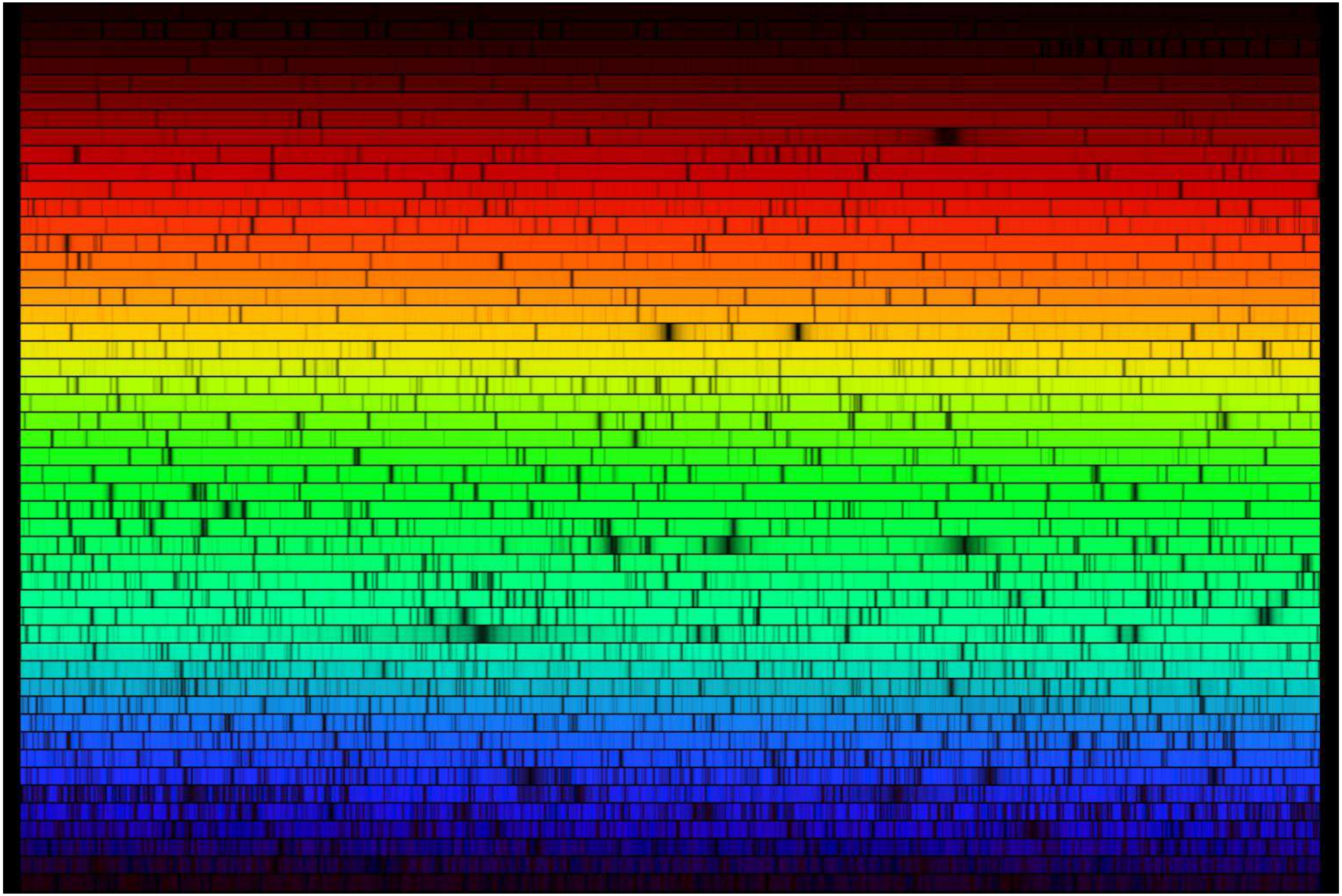
Atomic Spectra in Astrophysics



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Helium Spectra

He is the second-most abundant element: 25% by mass of the Universe atomic matter

HeI has -- electrons; HeII has -- electrons; HeIII has -- electrons.

α-particles formed during radioactive dfecay are ?

What is the wavelengths of Lα line in of HeII?

Selection rules for Complex Atoms

Strong transitions are driven by electric dipoles. Electric dipole selection rules are two types: rigorous rules - must always be obeyed; propensity rules - lead to weaker transitions.

Rigorous selection rules

(1) ΔJ must be 0 or +/- 1 with J = 0 - 0 forbidden

(2) $\Delta M_J = 0, +/- 1$

(3) Laporte rule: parity must change

Propensity selection rules

Additional set of rules which is not rigorously satisfied by complex atoms.

(4) The spin multiplicity is unchanged, $\Delta S=0$

(5) Only one electron jumps: the configuration of the two states must differ by only the movement of a single electron - Δn any, $\Delta l=+/-1$.

- Is $2s^2$ - $2s2p$ allowed? Is $2s^2$ - $2s3d$ allowed? Is $2s^2$ - $3p^2$ allowed?

Configuration interaction weakens this rule: e.g. ground state of Be $1s^2 2s^2$ is in fact mixed with 5% contribution from $1s^2 2p^2$

(6) $\Delta L=0, +/- 1$, $L=0$ 0 - 0 is forbidden.

- Is ^1S - $^1P^o$ allowed? And is ^3D - $^3P^o$ allowed? What about ^1S - $^1S^o$ allowed? And ^3S - $^3D^o$?

Table 5.1 Selection rules for atomic spectra. Rules 1, 2 and 3 must always be obeyed. For electric dipole transitions, intercombination lines violate rule 4 and forbidden lines violate rule 5 and/or 6. Electric quadrupole and magnetic dipole transitions are also described as forbidden.

	Electric dipole	Electric quadrupole	Magnetic dipole
1.	$\Delta J = 0, \pm 1$ Not $J = 0 - 0$	$\Delta J = 0, \pm 1, \pm 2$ Not $J = 0 - 0, \frac{1}{2} - \frac{1}{2}, 0 - 1$	$\Delta J = 0, \pm 1$ Not $J = 0 - 0$
2.	$\Delta M_J = 0, \pm 1$	$\Delta M_J = 0, \pm 1, \pm 2$	$\Delta M_J = 0, \pm 1$
3.	Parity changes	Parity unchanged	Parity unchanged
4.	$\Delta S = 0$	$\Delta S = 0$	$\Delta S = 0$
5.	One electron jumps Δn any $\Delta l = \pm 1$	One or no electron jumps Δn any $\Delta l = 0, \pm 2$	No electron jumps $\Delta n = 0$ $\Delta l = 0$
6.	$\Delta L = 0, \pm 1$ Not $L = 0 - 0$	$\Delta L = 0, \pm 1, \pm 2$ Not $L = 0 - 0, 0 - 1$	$\Delta L = 0$

Intercombination lines

Photons do not change spin → usual rule $\Delta S=0$. However, relativistic effects mix spin states, specially for high Z ions. Weak spin changing transitions → *intercombination lines*. Example: CIII] $2s^2\ ^1S$ - $2s2p\ ^3P^o$ at λ 1908.7Å

C^{2+} $2s2p\ ^3P^o$ state is *metastable* - no allowed radiative decay. Useful information about density.

Forbidden lines

Forbidden lines are, generally, weaker than intercombination lines.

(5) Only one electron jumps: the configuration of the two states must differ by only the movement of a single electron - Δn any, $\Delta l=+/-1$.

(6) $\Delta L=0$, +/- 1, L=0 0 - 0 is forbidden.

Electric dipole transitions which violete rules 5 and 6 - *forbidden transitions*.

1906.7 Å C[III] $2s^2\ ^1S_0$ - $2s2p\ ^3P^o_2$

322.57 Å C[III] $2s^2\ ^1S_0$ - $2p3s\ ^1P^o_1$

Even the rigorous selection rules can be modified when nuclear spin effects are taken into account.

ΔF must be 0, +1,-1, F=0-0 forbidden

Grotrian Diagrams

Walter Grotrian (1890-1954) - war erst Privat-Dozent an der Universität Potsdam. 1928 “Graphische Darstellung der Spektren”

(1) The vertical scale is energy. It starts from the ground state at zero, and extends to the first ionization limit. Sometime the binding energy, expressed relative to the first ionization limit, is given at the right side.

(2) Terms (levels) are represented by horisontal lines

(3) States with the same term (or level if fine structure effects are large), are stacked veritically and labeled by n of the outer electron.

(4) Terms are grouped by spin multiplicity.

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(5) States are linked by observed transitions with numbersw giving the wavelengths of the transition in Å. Thicker lines denote stronger transitions. Forbidden lines are given by dashed lines.

Lets construct Grotrian Diagram for HeI

Partial Grotrian Diagram for HeI

We need to know:

(1) Ionizattion potential HeI (what about HeII?). see e.g. NIST Database
https://dept.astro.lsa.umich.edu/~cowley/ionen.htm

(2) Terms (levels) are represented by horisontal lines: HeI terms ?

(3) How to arrange them in energy? Which rules regulate this?

(4) Terms are grouped by spin multiplicity.

(4) Allowed and forbidden transitions, wavelengths or wavenumbers

Lets construct Grotrian Diagram for HeI

Helium atom

1) The ground state $1s^2$. This is a closed shell, with L=, S=,

2) The first excited configuration is 1s2s. what are the terms?

Hund's rule: *For a given configuration, the state with the maimum spin multiplicity is lowest in energy.*

3) The next excited configuration 1s2p. Write levels and terms

Draw Grotrian diagram

The helium atom

1) The ground state $1s^2$. This is a closed shell, with $L=0$, $S=0$, hence it gives rise to a single, even parity term ^1S, and level $^1S_0$.

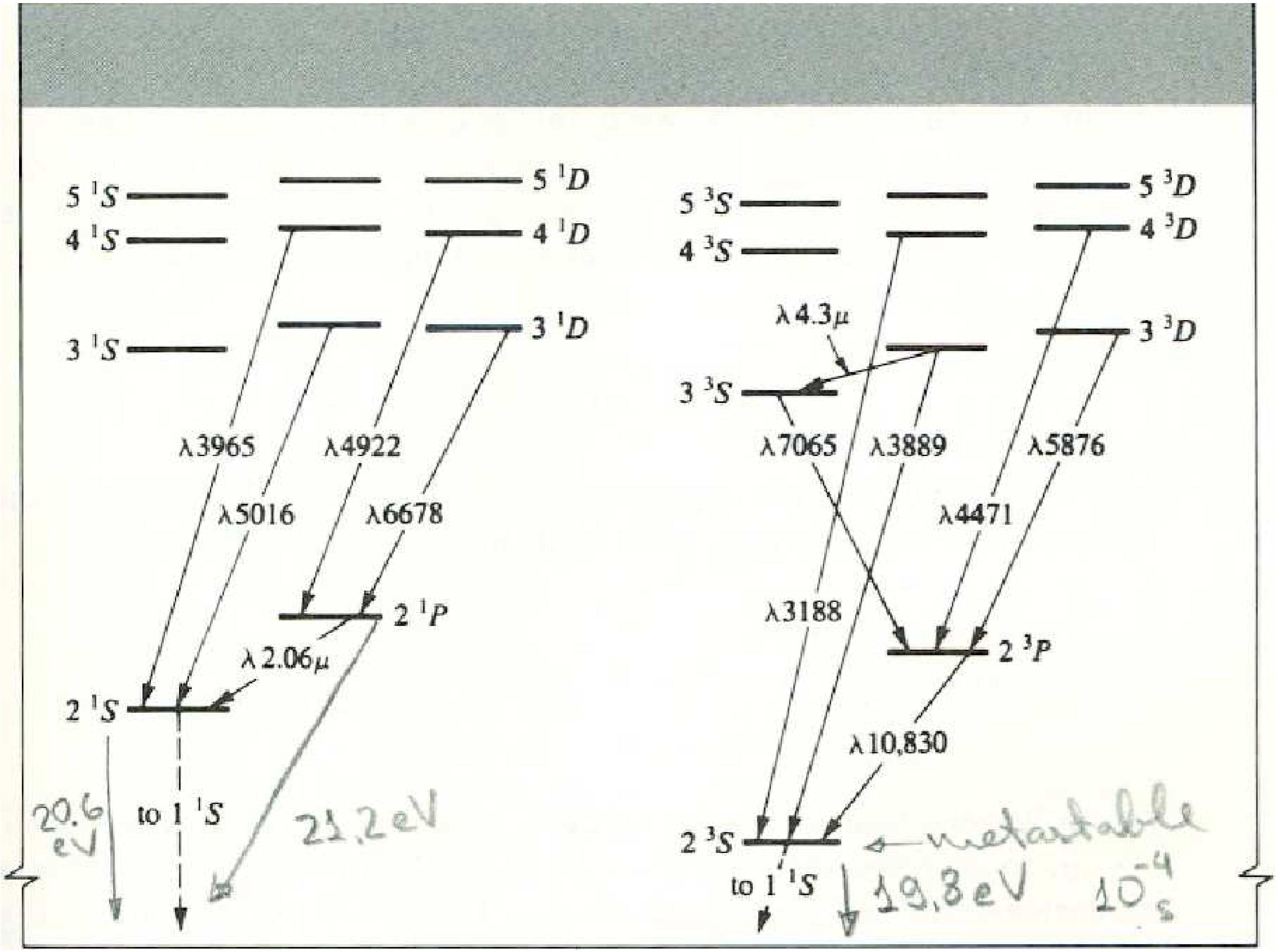
2) The first excited configuration is 1s2s. This has $l_1=l_2=0$ and hence $L=0$. But $S=0, 1$ giving rise to *singlets* and *triplets*.

Hund's rule: *For a given configuration, the state with the maimum spin multiplicity is lowest in energy.*

So the ^3S term ($^3S_1$ level) is lower in energy that the ^1S term ($^3S_0$ level). The spliting beween these terms is 0.8 eV.

3) The next excited configuration 1s2p. It has odd parity. $L=1$, $S=0, 1$. The $^3P^o$ term is lower than the $^1P^o$ term, in this case by 0.25 eV. The $^3P^o$ term splits into three levels: $^3P^o_0$, $^3P^o_1$, $^3P^o_2$

Partial energy diagram of He I, showing strongest optical lines



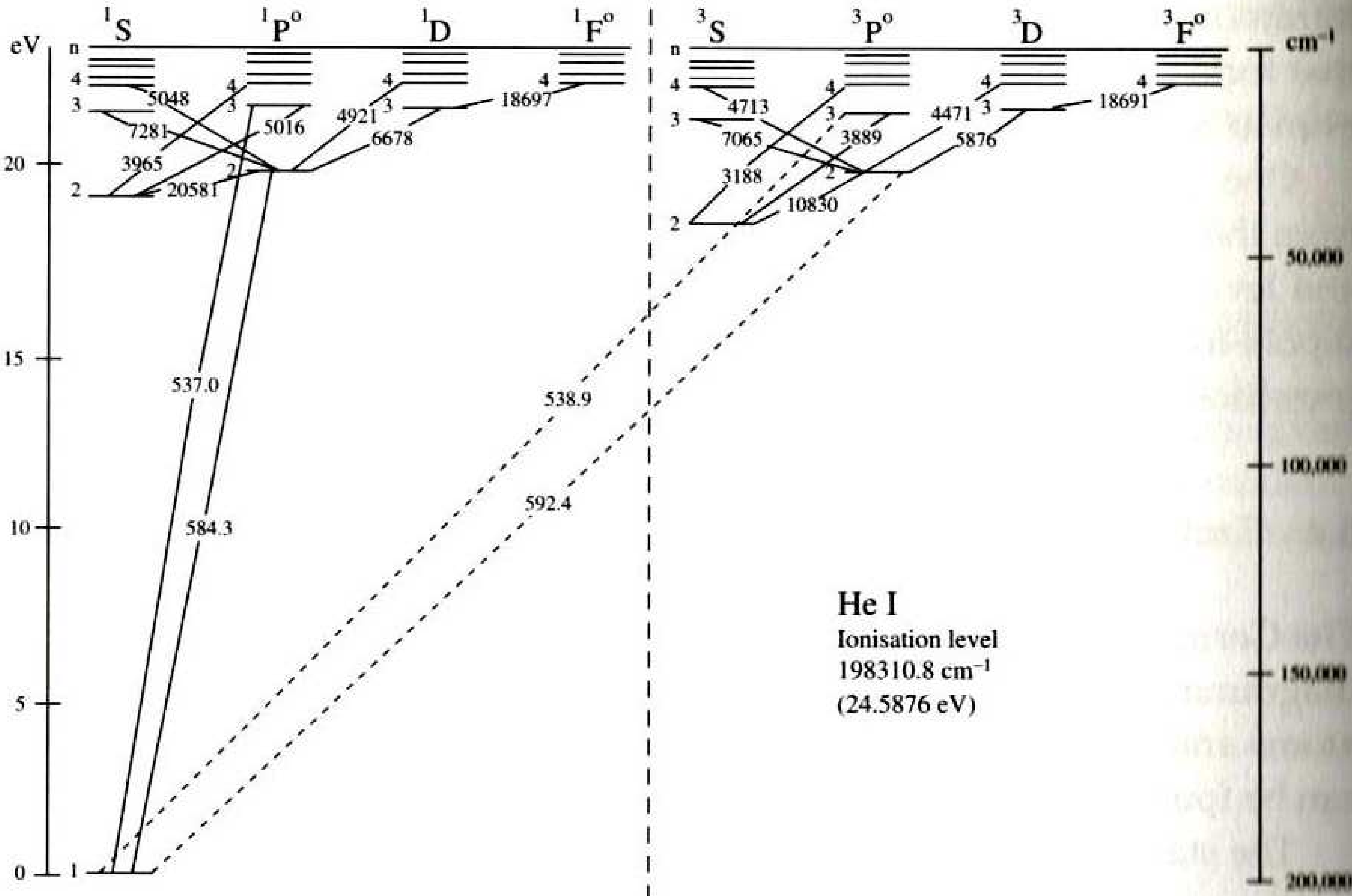
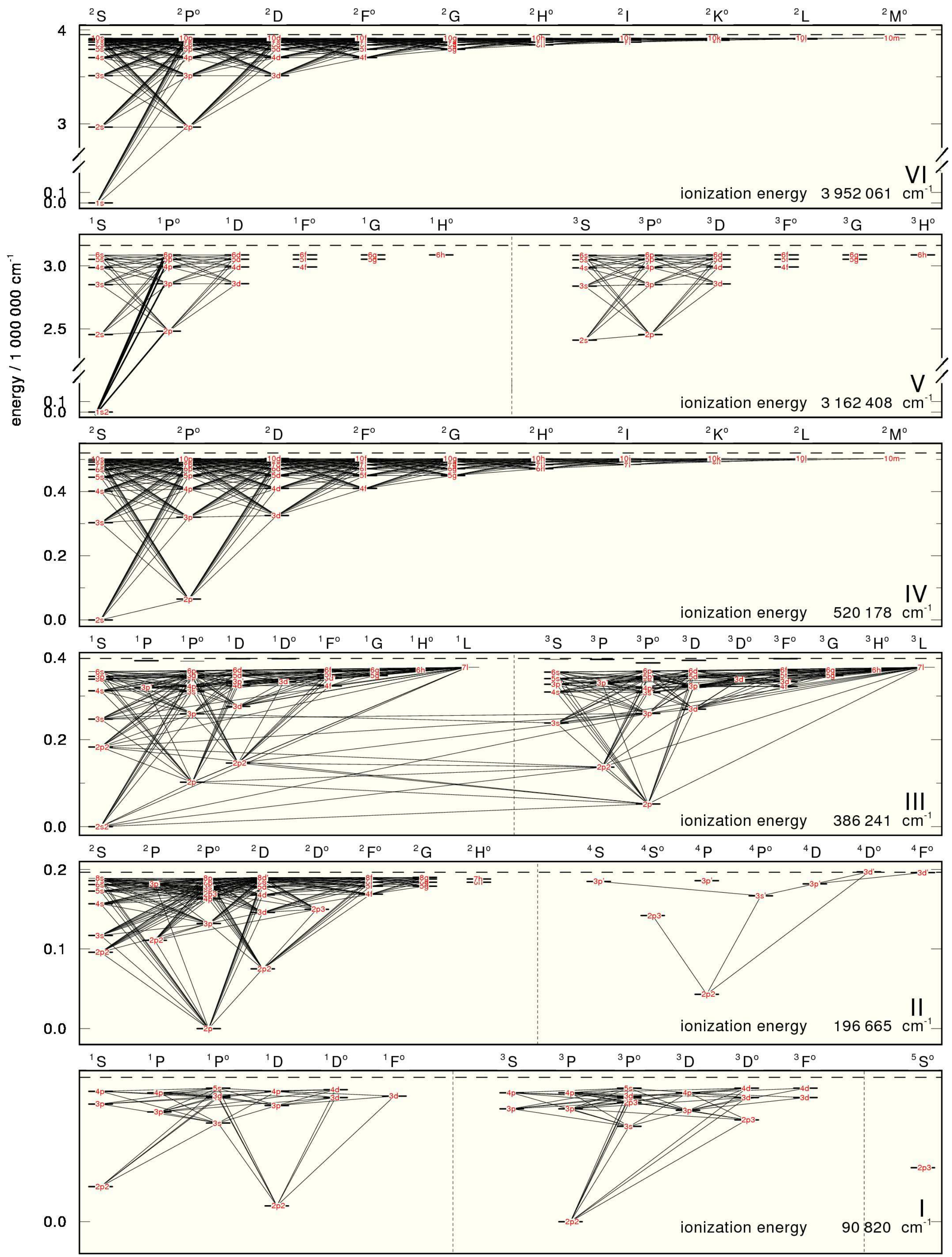


Fig. 5.2 Grotrian diagram for He I. The running numbers denote the principal quantum number of the active electron. The left-hand side of the figure is for 'para' singlet helium and the right-hand side is for 'ortho' triplet helium.

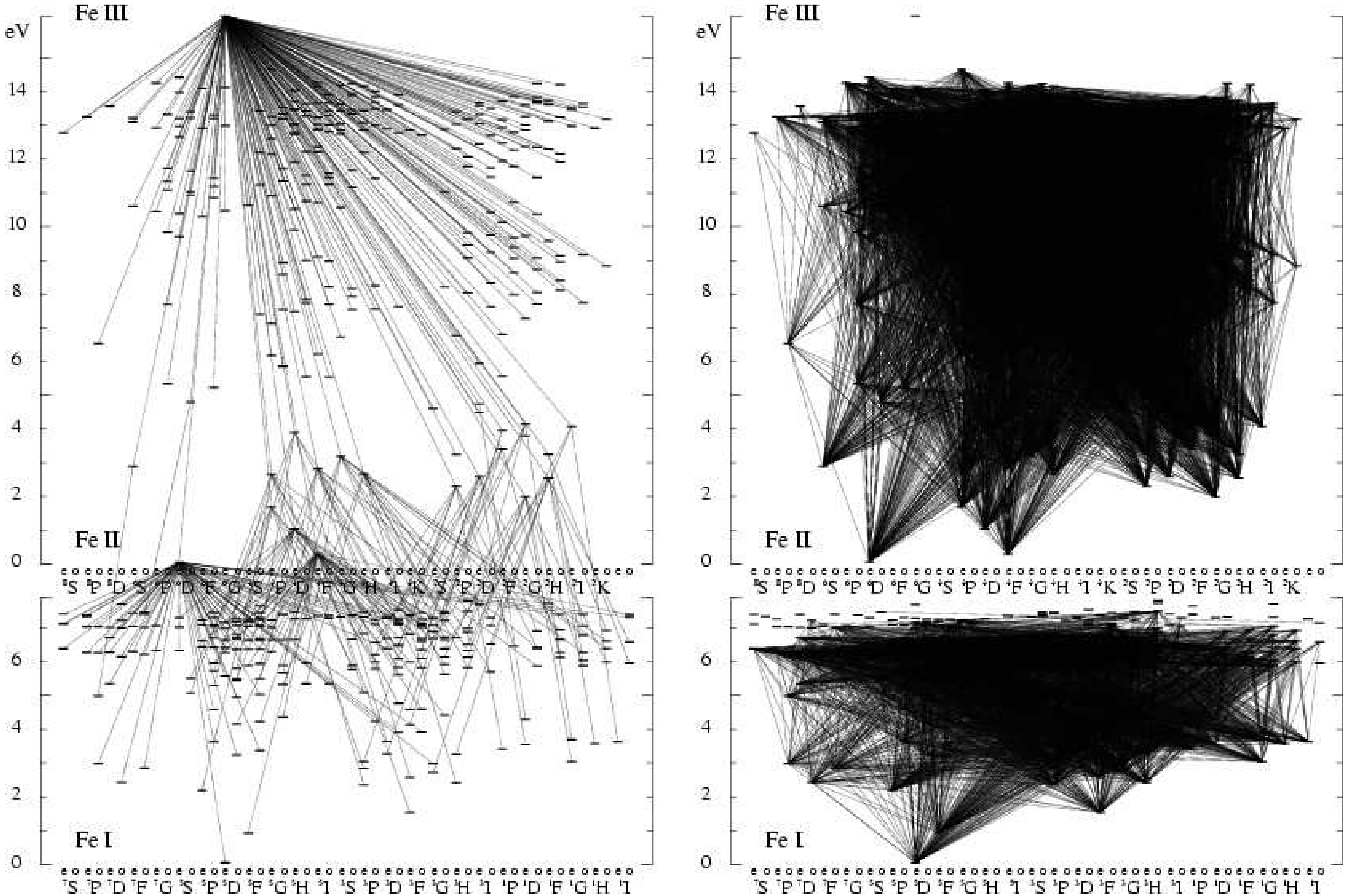


Grotrian diagrams are powerful spectroscopic tool

Different resources exist

https://ned.ipac.caltech.edu/level5/Ewald/Grotrian/frames.html

Carbon Grotrian diagrams
Level energies are from NIST (thick horizontal lines) or OPACITY PROJECT (thin lines).
Line transitions are from OPACITY PROJECT.
Model atoms are provided by TMAD (http://astro.uni-tuebingen.de/~TMAD/TMAD.html) in the framework of GAVO (http://www.g-vo.org/).


Fe III
eV
Fe II
Fe I
Fe III
eV
Fe II
Fe I

Exercise 1

Emission of HeII are observed ay 1640Å. To what transitions does this radiation corresponds to? What other emission lines are expected in this spectrum?

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HeII $\frac{1}{\lambda} = 4R_{\mathrm{He}}(\frac{1}{n_1^2} - \frac{1}{n_2^2}) = R_{\mathrm{He}}(\frac{1}{(n_1/2)^2} - \frac{1}{(n_2/2)^2})$

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1640Å corresponds to Balmer α with n=3-2. One expects Lyβ n=3-1 λ 256Å and Lyα λ 304Å.

Exercise 2

The He-like NVI is formed in the hot intergalactic medium with configurations 1s2s and 1s2p.

1) What levels can be formed from these configurations?
2) By what mechanism would you expect each level to transit to $1s^2$ ground state?
3) Order these transitions according to their approximate strengths.

Exercise 2

The He-like NVI is formed in the hot intergalactic medium with configurations 1s2s and 1s2p.

1) What levels can be formed from these configurations?

1s2s has $l_1 = l_2 = L = 0$ and $s_1 = s_2 = 1/2$ → ${}^1S_0$ and ${}^1S_1$

1s2p has l_1; $l_2 = 1$; $L = 1$ and $s_1 = s_2 = 1/2$ → $S = 0, 1$

1s2p has odd parity. $L=1$, $S=0, 1$. The ${}^3P^o$ term is lower than the ${}^1P^o_1$ term. The ${}^3P^o$ term splits into three levels: ${}^3P^o_0$, ${}^3P^o_1$, ${}^3P^o_2$

Exercise 2

The He-like NVI is formed in the hot intergalactic medium with configurations 1s2s and 1s2p.

2)Possible transitions to ground state

1s2s has $l_1=l_2=L=0$ and $s_1=s_2=1/2$ → $^1S_0$ and $^1S_1$

1s2p has l_1; $l_2=1$; $L=1$ and $s_1=s_2=1/2$ → $S=0,1$

1s2p has odd parity. $L=1$, $S=0, 1$. The $^3P^o$ term is lower than the $^1P^o_1$ term. The $^3P^o$ term splits into three levels: $^3P^o_0$, $^3P^o_1$, $^3P^o_2$

1s2p-$1s^2$ $^1P^o_1$-$^1S_0$ resonace line

1s2p-$1s^2$ $^3P^o_1$-$^1S_0$ intercombination line

1s2p-$1s^2$ $^3P^o_2$-$^1S_0$ magnetic quadrupole line

1s2p-$1s^2$ $^3S_1$-$^1S_0$ spin-forbidden magnetic transition

The two $J=0$ levels cannot decay to the ground state transitions while $J=0$-0 does not occur in any selection rules

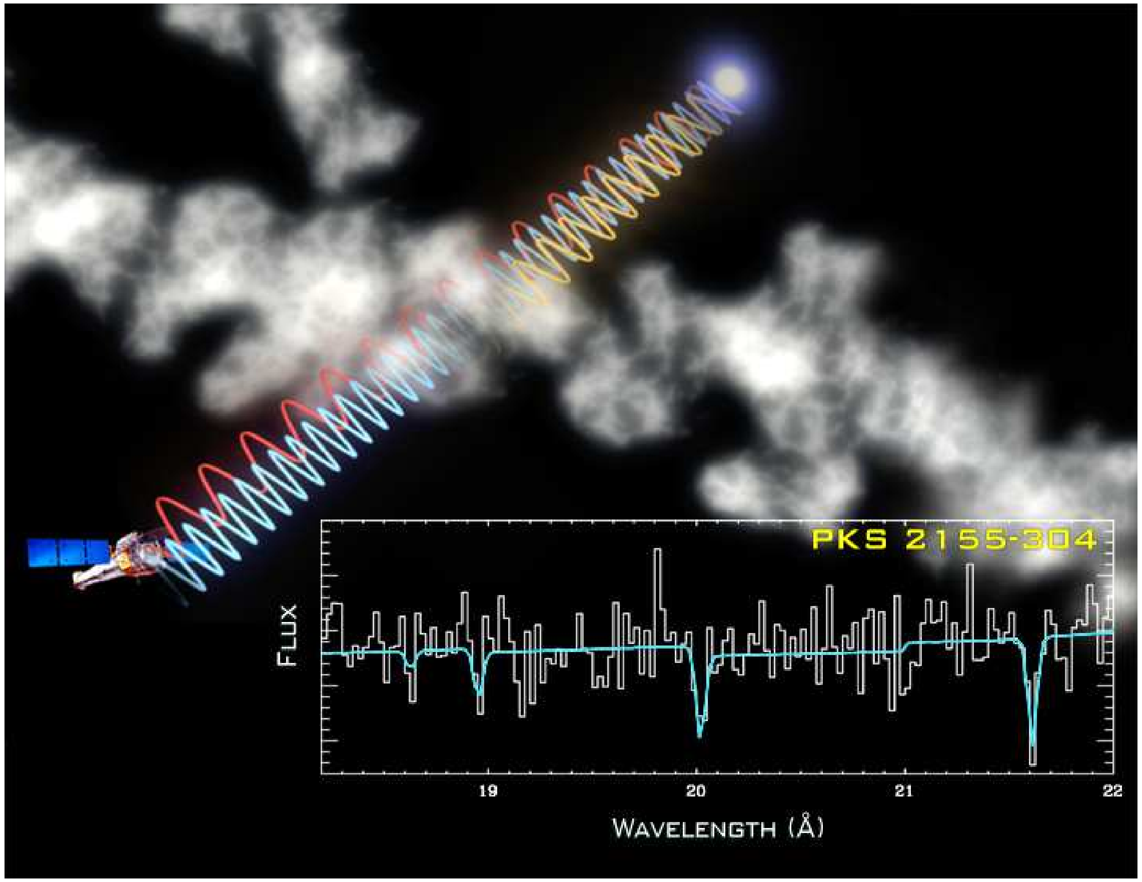
Exercise 2

The He-like NVI is formed in the hot intergalactic medium with configurations 1s2s and 1s2p.

What is ionization potential of NI-> NVI?

https://dept.astro.lsa.umich.edu/~cowley/ionen.htm

Warm-Hot Intergalactic Medium and a Missing Barion problem

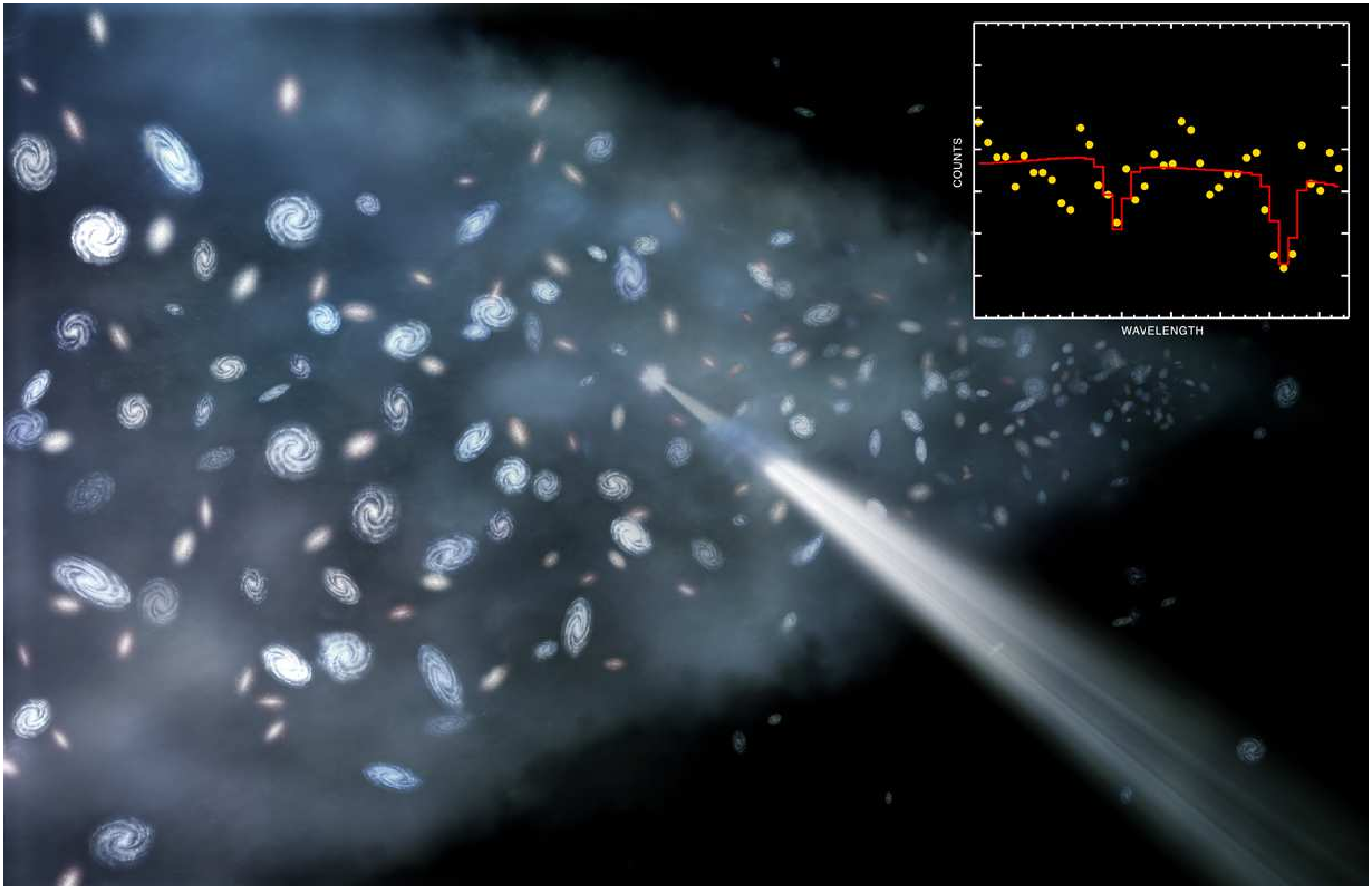


NASA/CXC/A.Hobart; Spectrum: NASA/MIT/T.Fang et al.

The total amount of the luminous baryons in the nearby universe probed by the stellar light, narrow Lyα absorption, as well as the X-ray emission from the hot intracluster and intragroup medium, accounts for at most 50% of the total baryonic matter in the low-redshift universe (e.g., Fukugita et al. 1998).

Large-scale, cosmological hydrodynamic simulations predict that most of the missing baryons are distributed as filamentary structures between galaxies, in the form of a warmhot interintergalactic medium WHIM with $T=10^5$-10^7 K

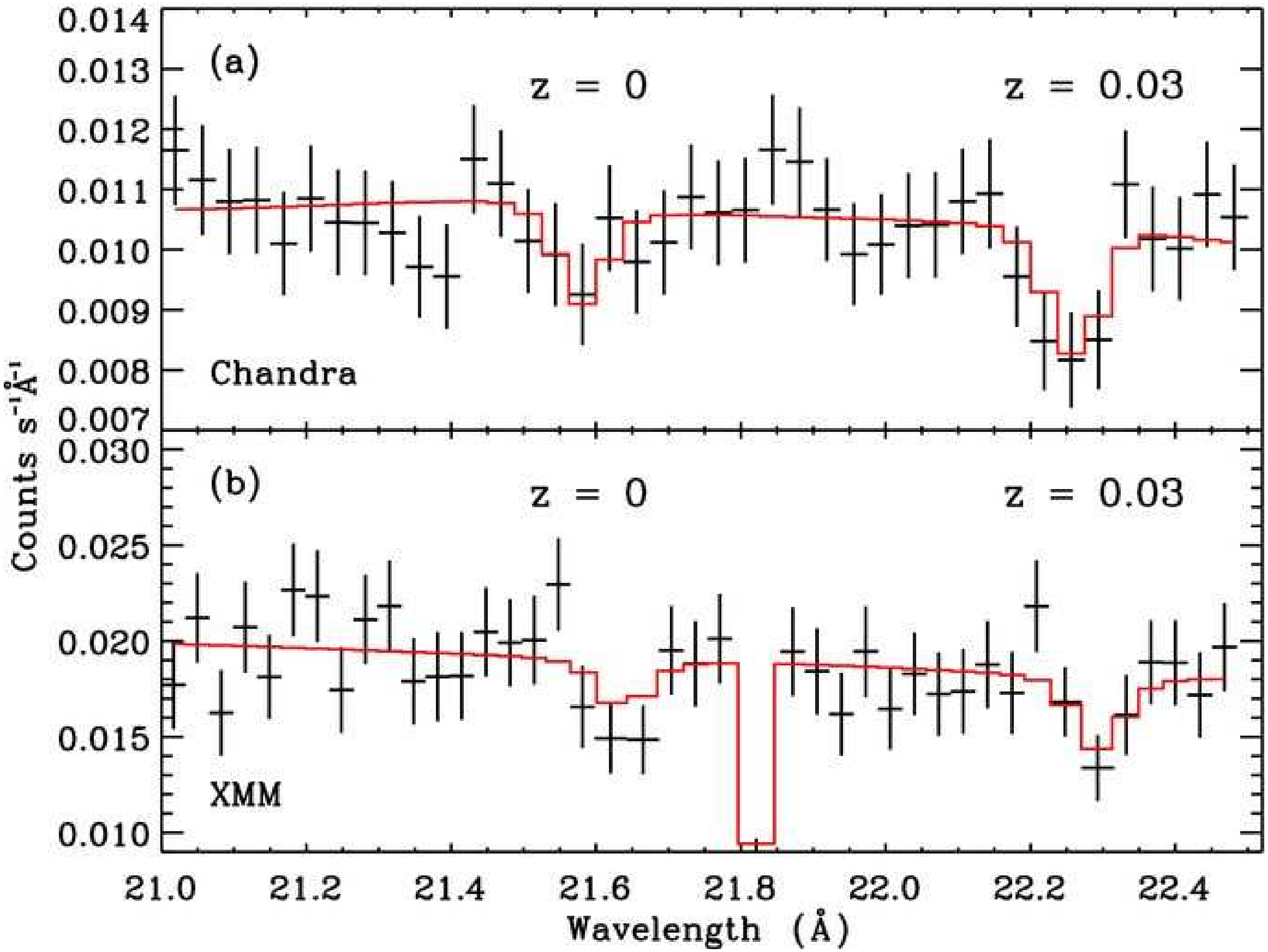
Warm-Hot Intergalactic Medium and a Missing Barion problem



NASA/CXC/M.Weiss;NASA/CXC/Univ. of California Irvine/T. Fang et al.

Present of absorption lines is confirmed by both Chandra and XMM-Newton observatories.

WHIM photoionizaed or collisional?

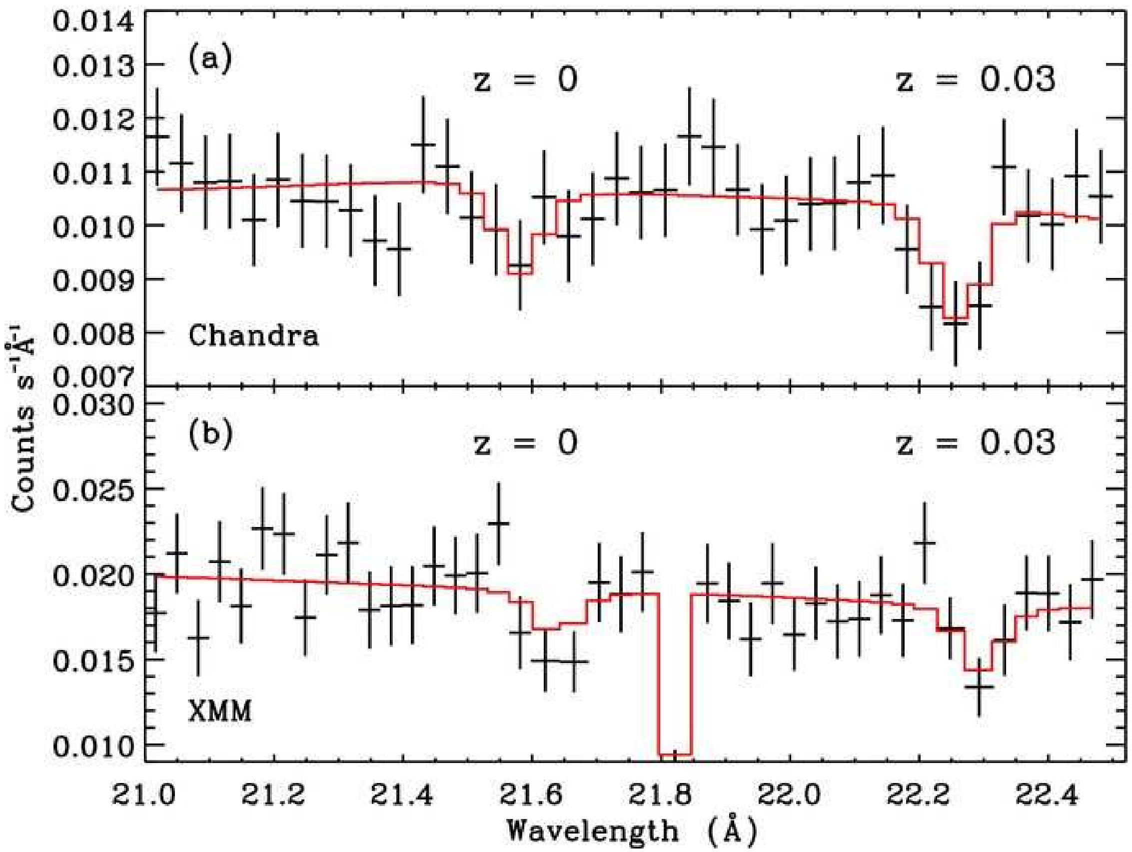


The Astrophysical Journal 714 (2010) 1715

OVII Kα absorption lines at the positions corresponding to the local (z=0) absorber and the Sculptor Wall (z=0.03)

To understand the properties of the absorber, we shall know how OVII is formed: photoionization or collisions.

WHIM photoionizaed or collisional?



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The cosmological simulations predict that WHIM gas at this over-density should have a temperature of approx. 1 MK. To estimate density we shall know ionization fraction of OVII vs. e.g. OVI

The OVI absorbers (FUV) probe the low-density, low-temperature portion of the WHIM because the OVI ionization fraction peaks near T= 3 10^5 K assuming collisional ionization. If the OVI absorbers are produced by photo-ionized gas, then the gas is even colder (T < 10^5 K). On the other hand, the WHIM gas probed by X-ray emission studies typically has a higher temperature (T=10^7 K) and higher over-density