Topic 1E - Many-Electron Atoms

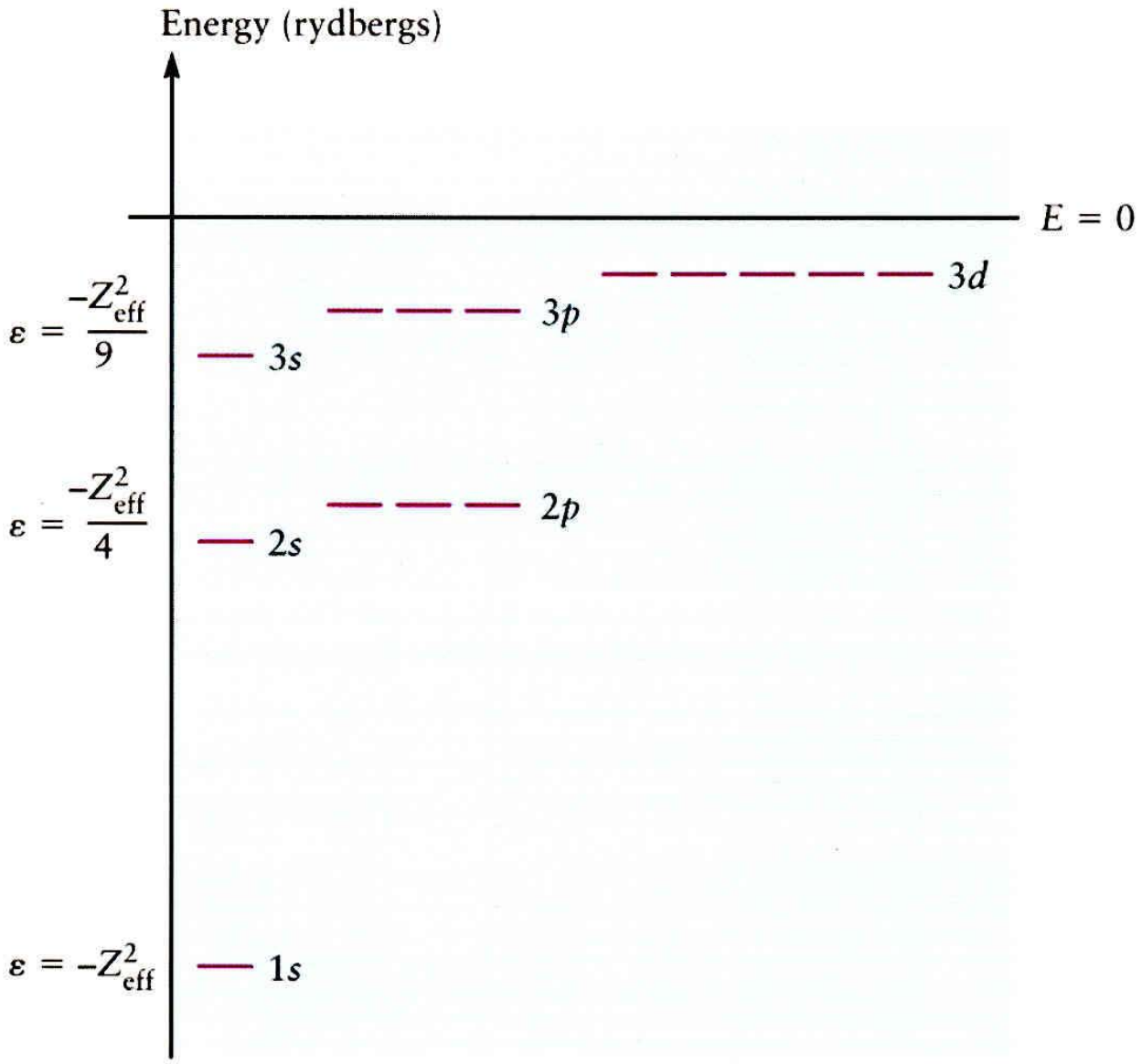
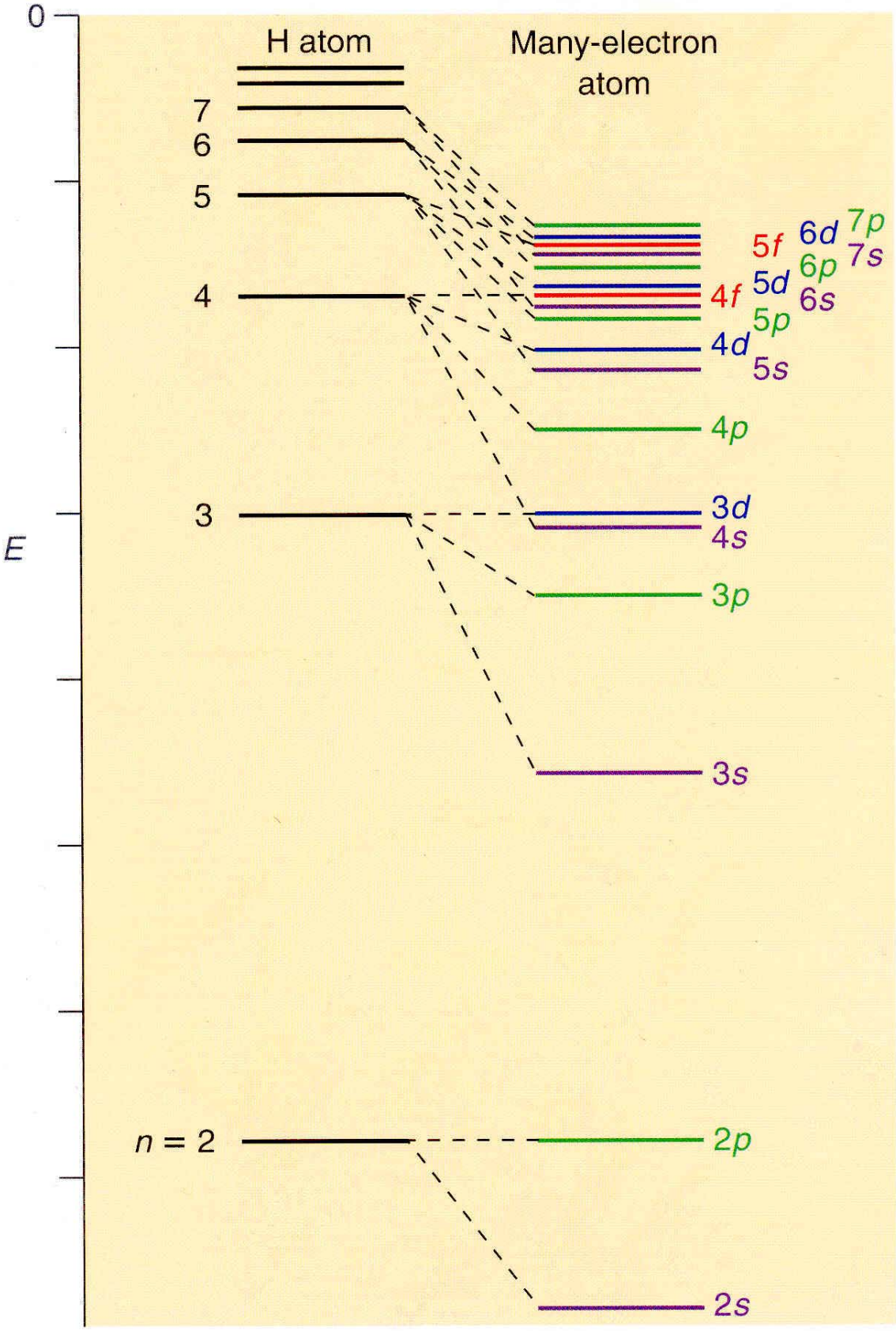


FIGURE 5.14 Approximate energy-level diagram for Hartree orbitals, estimated by incorporating values of Z_{eff}. Energy values are in units of rydbergs. The result of electron–electron repulsion is to remove the degeneracy of the hydrogen atom states with different ℓ values.

Figure 4.7: Splitting of Orbital Energies



Pauli Exclusion Principle

In a given atom, no two electrons can have the same set of four quantum numbers, n, ℓ, m_ℓ, and m_s.

A single orbital (*i.e.*, energy state) in a given atom can be occupied by, at most, two electrons, if they have opposite spin states.

(More generally, two electrons having the same spin state may not occupy the same point in space at the same time.)

Hund's Rule

The lowest-energy electronic configuration in a given atom is the one having the maximum number of unpaired electrons allowed by the Pauli Principle in a particular set of degenerate orbitals.

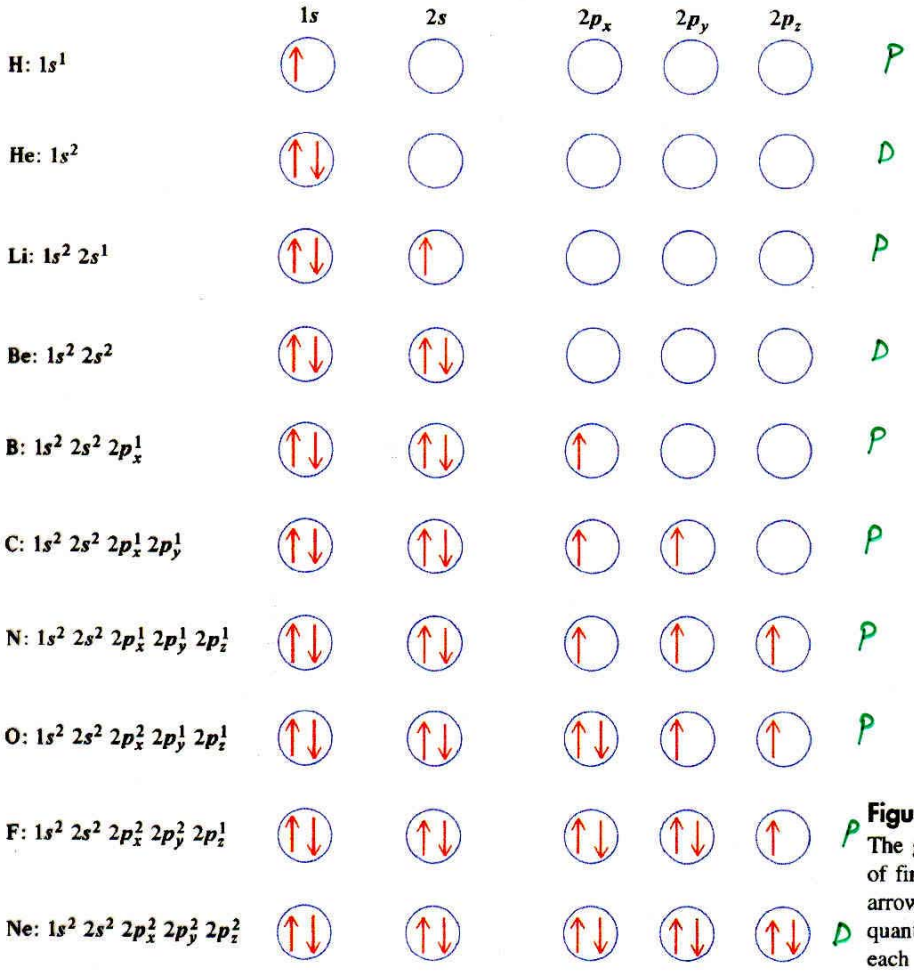
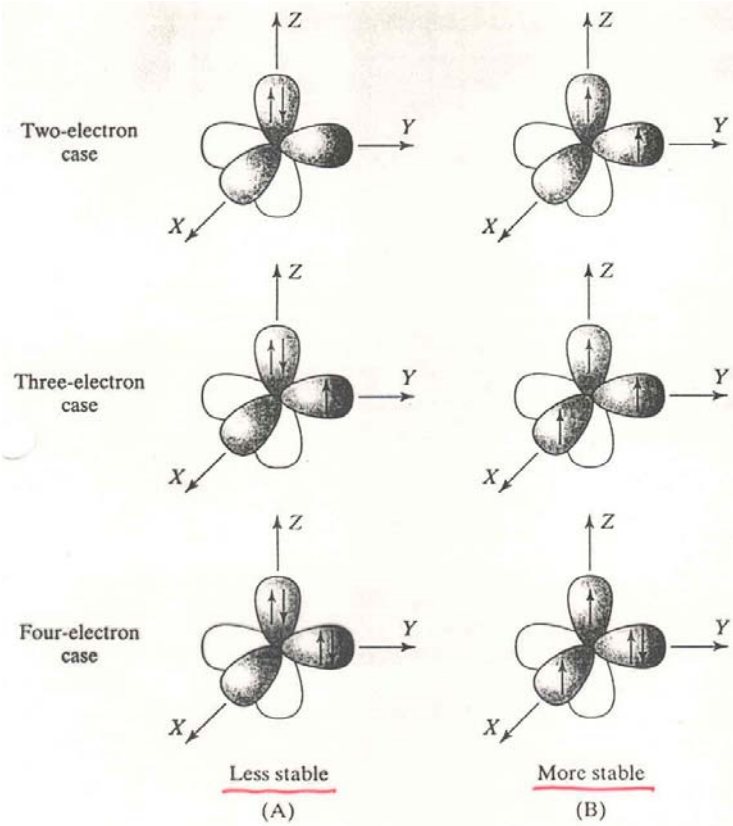


Figure 13-25
The ground-state electron configurations of first- and second-period atoms. The arrows represent electrons with spin quantum numbers $m_s = +\frac{1}{2}$ or $m_s = -\frac{1}{2}$; each circle represents an orbital.



◀ FIGURE 13.20
Qualitative illustration of the additional stability produced by placing electrons in different degenerate orbitals when permitted by the Pauli principle. In (A), for the two-, three-, and four-electron cases, one or more spatial *p*-orbital contains two electrons. The electrons are, therefore, in close proximity, with the result that their mutual repulsion is large. In (B), the electrons are placed in different degenerate spatial orbitals, thereby minimizing their mutual repulsion, which results in a more stable arrangement. The shaded lobe of the orbitals point in the positive direction. Arrows indicate electrons, with the direction of the arrow specifying the spin orientation.

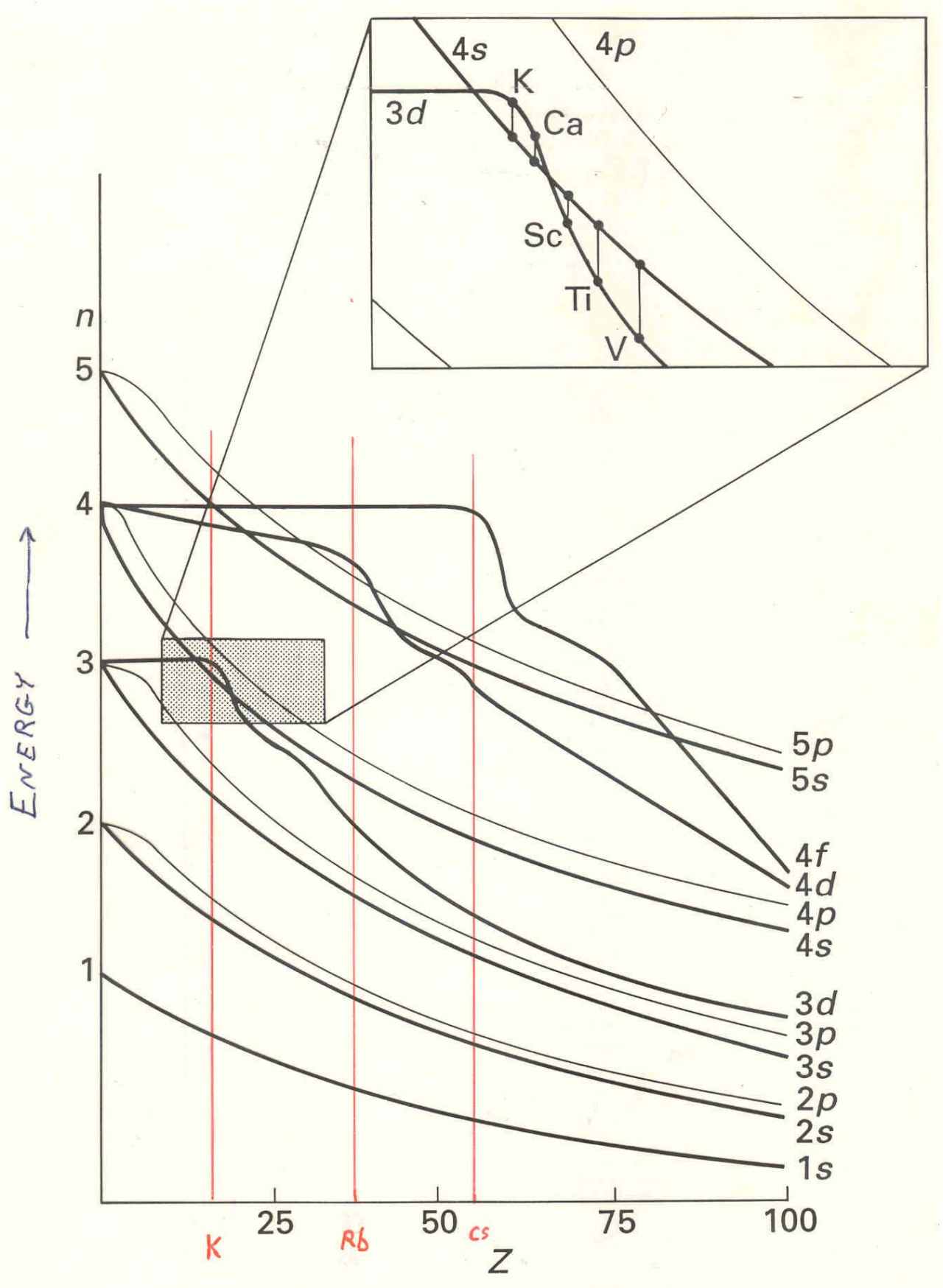

4s
4p
K
3d
Ca
Sc
Ti
V
n
5
4
3
2
1
ENERGY
5p
5s
4f
4d
4p
4s
3d
3p
3s
2p
2s
1s
25
50
75
100
K
Rb
Cs
Z

Table 4.2: Anomalous Electron Configurations

TABLE 4.2

Anomalous electron configurations*

Period	Z	Element	Configuration	Period	Z	Element	Configuration
4	24	Cr	$[Ar]4s^1 3d^5$	6	57	La	$[Xe]6s^2 5d^1$
4	29	Cu	$[Ar]4s^1 3d^{10}$	6	58	Ce	$[Xe]6s^2 4f^1 5d^1$
5	41	Nb	$[Kr]5s^1 4d^4$	6	64	Gd	$[Xe]6s^2 4f^7 5d^1$
5	42	Mo	$[Kr]5s^1 4d^5$	6	78	Pt	$[Xe]6s^1 4f^{14} 5d^9$
5	44	Ru	$[Kr]5s^1 4d^7$	6	79	Au	$[Xe]6s^1 4f^{14} 5d^{10}$
5	45	Rh	$[Kr]5s^1 4d^8$	7	89	Ac	$[Rn]7s^2 6d^1$
5	46	Pd	$[Kr]4d^{10}$	7	90	Th	$[Rn]7s^2 6d^2$
5	47	Ag	$[Kr]5s^1 4d^{10}$	7	91	Pa	$[Rn]7s^2 5f^2 6d^1$
				7	92	U	$[Rn]7s^2 5f^3 6d^1$

* These configurations cannot be deduced by following the Aufbau ordering indicated in Figure 4.5, with the possible exception of La and Ac, where these elements are retained in the *d* series.